

GURU Package Manual

Overview

The **GURU** package is a collection of tools for post-processing molecular dynamics and ab initio simulation data.

It currently includes four main modules:

1. **guru-thermo** — extract and average thermodynamic properties from VASP OUTCAR or legacy logs.
2. **guru-iso-fit** — fit isotherm/isochor curves with polynomials and find reference states.
3. **guru-hugoniot** — compute Hugoniot shock adiabat points along isotherms and isochors.
4. **guru-tsv-cat** — concatenate TSV tables produced by other modules, keeping header only once.

Each module is installed as a CLI entry point (`guru-thermo`, `guru-iso-fit`, `guru-hugoniot`, `guru-tsv-cat`).

1. guru-thermo

Purpose

Parse VASP `OUTCAR` (or legacy per-step logs) to extract energies, pressures, and temperatures, and compute averages with statistical error estimates.

Usage

```
guru-thermo -i OUTCAR --skip 500 --end 2000 --out averages.tsv --dump-log ep_log.tsv
```

Options

`-i, --input` : Input file (`OUTCAR` or log).
`--skip` : Skip first N steps (default: 0).
`--end` : End index for averaging (default: until EOF).
`--maxrows` : Maximum number of rows to use after skipping.
`--strict` : Warn/fail if missing values are encountered.
`--out` : Write detailed averages with variance and density.
`--dump-log` : Dump per-step thermo log.

Output

Compact stdout:

T P E

...

Optional TSV with mean, std error, variance, and structure info (cell volume, density).

2. guru-iso-fit

Purpose

Fit isotherms (constant T , varying ρ) or isochors (constant ρ , varying T) using polynomial regression. Used to determine reference states for Hugoniot.

Usage

```
guru-iso-fit --mode isotherm --degree 2 --pressure 100 -i data1.tsv data2.tsv -o ref.tsv --plot
```

Options

`--mode {isotherm, isochor}` : Select fitting mode.
`--degree`` : Polynomial degree (1, 2, or 3).
`--pressure`` : Target pressure for solving curve.
`--tol`` : Tolerance for uniformity check (default: 10 for isotherm, 0.01 for isochor).
`--on-outliers {warn, ignore, fail}`` : Outlier handling strategy.
`--plot`` : If set, also generates PNG plots with fit curves and selected points.

Output

TSV containing the evaluated point on the fitted curve, with P , E , T , ρ and flags.

3. guru-hugoniot

Purpose

Compute Hugoniot shock adiabat points from thermo data and a reference state.

Usage

```
guru-hugoniot --initial ref.tsv --Ma 27.0 -i T*.tsv -o hugoniot.tsv
```

Options

`--initial`` : TSV file with reference state (from iso-fit or guru-thermo).

`--Ma`` : Molar mass in g/mol.
`--rho0`` : Reference density if not present in initial TSV.
`-i, --input`` : Input thermo TSV files.
`--group-dT`` : Temperature grouping tolerance (K) for isotherms.
`--group-drho`` : Density grouping tolerance (g/cm³) for isochors.
`--curves {iso, rho, both}`` : Which curve families to process.
`--interp {linear, pchip}`` : Interpolation method.

Output

TSV with columns:

``curve_type``
``label``
``P[kbar]``
``T[K]``
``rho[g/cm^3]``
``is_extrapolated``
``rho/rho0``
``D[km/s]`` (shock velocity)
``U[km/s]`` (particle velocity)

4. guru-tsv-cat

Purpose

Concatenate multiple TSV tables into one, keeping the header only once.

Usage

`guru-tsv-cat -o merged.tsv file1.tsv file2.tsv ...`

Output

Merged TSV with consistent header.

Common Formats for Manuals

Besides **Markdown (.md)** and **PDF**, software manuals are also commonly distributed in:

reStructuredText (.rst) — used in Python ecosystem and Sphinx docs.

HTML — rendered web manuals.

man pages (``groff`/`troff`` format) — for UNIX CLI tools.

LaTeX/PDF — scientific/technical reports.

EPUB — portable e-book format.