User Guide for GTS

GTS: A Python toolkit for building Gibbs thermodynamic surface with application to obtain high-pressure melting data

Version: 1.0.4

Overview

GTS: Gibbs Thermodynamic Surface is an automated toolkit designed for efficiently obtaining high-pressure melting data, including melting points and thermodynamic potentials of materials. By constructing the Gibbs thermodynamic surface using a geometrical method, it provides fast and accurate calculations for both solid and liquid phases.

Features

- **Automated surface generation**: Builds thermodynamic surfaces for solid and liquid phases.
- **Melting data**: Obtaining melting data for solid and liquid phases based on user-defined pressure conditions. With the *ab initio* molecular dynamics (AIMD) simulation data in the NVT (N, number of atoms; V, volume; T, temperature) ensemble and the reference point, GTS is able to rapidly present melting data, including volume, pressure, temperature, and thermodynamic potentials
- **A reference point**: Comparing the traditionally-used Clausius-Clapeyron integration (CCI) method with our GTS approach, the same thing is that a reference melting point is needed.

Installation

From PyPI

You can install GTS directly from PyPI: **`pip install GibbsTS`**

From Source

1. Clone the repository:

```
git clone https://github.com/computation-mineral-physics-group/GTS.git
```

2. Install dependencies:

```
pip install -r requirements.txt
```

3. Install GTS:

```
pip install .
```

Run

GTS provides two primary functions: **building the Gibbs thermodynamic surface** and **calculating melting data**. These functionalities can be accessed via a command-line interface.

Input Files

It is of great importance to prepare two files before running: **`{name}_solid_input.txt`**, **`{name}_liquid_input.txt`**.

Command For Running

Argument	Type	Default	Description
`n, --name`	str	None	Name of the material
`-s, --surface`	bool	False	Build thermodynamic surface and store its data in `[name].json`
`-mtr, -- melt_temp_refer`	float	0	The reference melting temperature (in K)
`-mpr, -- melt_pressure_refer`	float	0	The reference melting pressure (in GPa)
`-p, --pressure`	float	0	The target pressure for a melting point (in GPa)
`-i, --image`	bool	False	Save the G-T plot indicating the melting point
`-u, --unit`	str	internal	Units for the output (e.g., `vasp` or `internal`)
`-min, --minpressure`	float	0	Lower limit of the pressure range (in GPa)
`-max, --maxpressure`	float	0	Upper limit of the pressure range (in GPa)
`-num, --number`	int	6	Number of the melting points
`-d, --debug`	bool	False	Enable debug mode
`-v, --version`	Action	-	Show the program's version.
`-n, --name`	Action	-	Show the help message

Command line

1. Generate Thermodynamic Surface

Run the following command to generate the Gibbs thermodynamic surface for the target material and store the data in **`[name].json`**:

```
GTS -n [name] -s -mtr [value] -mpr [value]
```

2. Obtain Melting Data

This command will output the user-defined melting point and its thermodynamic potentials for the two phases (solid phase and liquid phase) in the terminal.

```
GTS -n [name] -p [value] -u [type] -i
```

This command will output the diagrams of thermodynamic potentials over the user-defined pressure range.

```
GTS -n [name] -min [value] -max [value]
```

3. Debug Model

In step I, GTS retains the original data for building primitive surfaces in two directories: **`{name}_solid`** and **`{name}_liquid`**. After entropy calibration, derived surface data is stored in **`twophase`**.
In step II, for a single user-defined pressure value, the fitting data is kept in the directory: **`{name}_{pressure_value}_melting_data`**, during obtaining melting data. For a user-defined pressure range, the fitting data is kept in the directory: **`{name}_{min}_{max}_melting_data`**.

Example

Here, we presented an example execution for periclase MgO. The input files and output surface data (JSON file) are presented in the directory: `.\doc\example`.

Step I

At the working directory which contain the two input files of GTS, execute the command line: **`GTS -s -n MgO -mtr 5915 -mpr 52`** (Fig. 1).

```
(base) zhaoxuan@DESKTOP-QQS359Q:~/GTS/test/MgO/example$ ls
MgO_liquid_input.txt  MgO_solid_input.txt
(base) zhaoxuan@DESKTOP-QQS359Q:~/GTS/test/MgO/example$ GTS -s -n MgO -mtr 5915 -mpr 52
```

Figure 1

Then GTS starts to build the thermodynamic surface (Fig. 2).

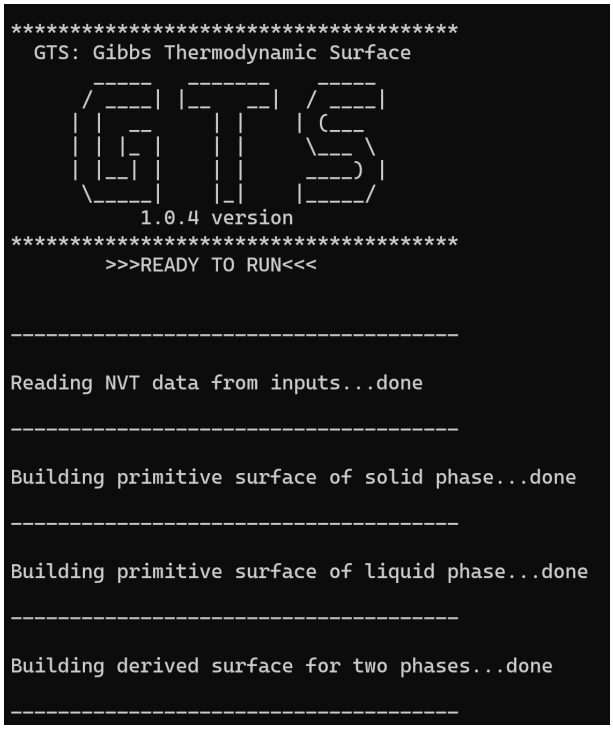

Figure 2

In debug mode, the fitting data will be stored in current working directory (Fig. 3 &4).

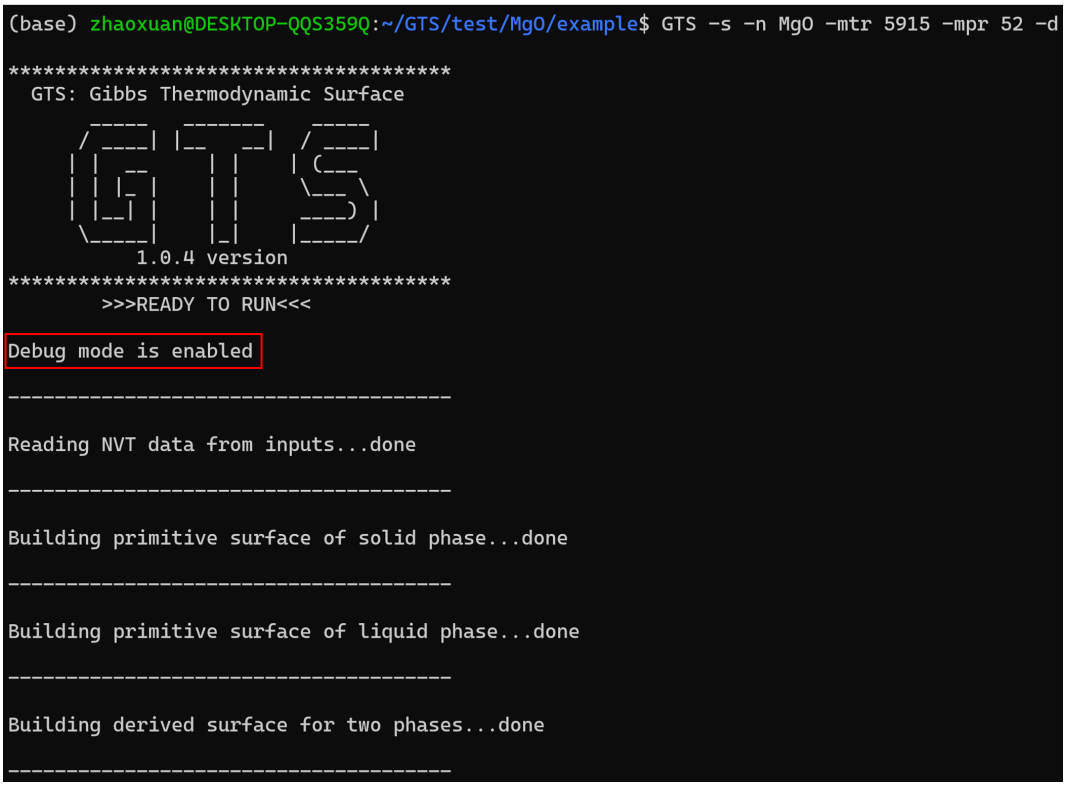

Figure 3

```
(base) zhaoxuan@DESKTOP-QQS359Q:~/GTS/test/MgO/example$ ls -l
total 1700
-rw-r--r-- 1 zhaoxuan zhaoxuan 1717353 Jul  2 16:41 MgO.json
drwxr-xr-x 2 zhaoxuan zhaoxuan    4096 Jul  2 16:39 MgO_liquid
-rw-r--r-- 1 zhaoxuan zhaoxuan    2397 Dec 18  2024 MgO_liquid_input.txt
drwxr-xr-x 2 zhaoxuan zhaoxuan    4096 Jul  2 16:39 MgO_solid
-rw-r--r-- 1 zhaoxuan zhaoxuan    1564 Dec 18  2024 MgO_solid_input.txt
drwxr-xr-x 3 zhaoxuan zhaoxuan    4096 Jul  2 16:41 twophase
```

Figure 4

Step II

If the user defined a single pressure value which is 110 GPa, execute the command line: **`GTS -n MgO -p 110 -i`** (Fig. 5). GTS will store the G-T plot (Fig. 6).

```
(base) zhaoxuan@DESKTOP-QQS359Q:~/GTS/test/MgO/example$ GTS -n MgO -p 110 -i

************************************
  GTS: Gibbs Thermodynamic Surface
       _____    _______    _____
      / ____| |__   __|  / ____|
     | |  __     | |    | (___
     | | |_ |    | |     \___ \
     | |__| |    | |     ____) |
      \_____|    |_|    |_____/
           1.0.4 version
************************************
        >>>READY TO RUN<<<


----------------------------------------

Obtaining the melting data...done

----------------------------------------

material_name       = MgO
melting_pressure    = 110.000 GPa
melting_temperature = 7451.2 K
 ####   #solid#  #liquid#     #units#
  G      1.463     1.460   1.0e-19 J/atom
  A     -6.482    -6.925   1.0e-19 J/atom
  H      0.746     2.201   1.0e-19 J/atom
  U     -7.199    -6.184   1.0e-19 J/atom
  S     -0.096     0.099  1.0e-22 J/K/atom
  V      0.722     0.762 1.0e-29 m**3/atom
Image saved at /home/zhaoxuan/GTS/test/MgO/example

----------------------------------------
```

Figure 5

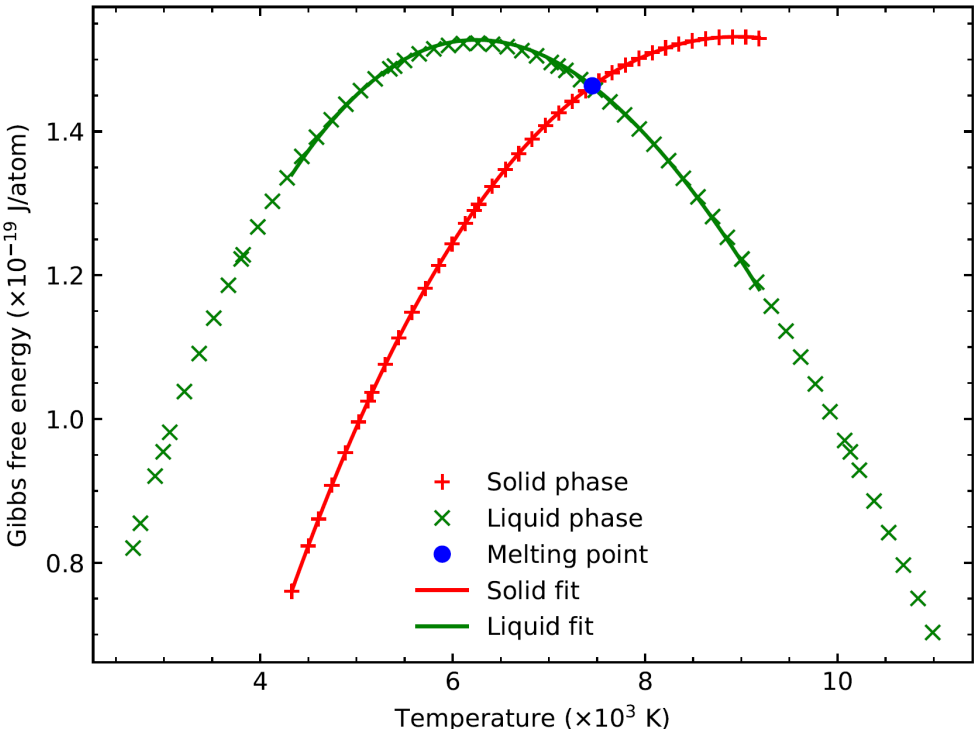

Figure 6

If the user defined a pressure range from 40 to 120 GPa, execute the command line: **`GTS -n MgO -min 40 -max 120`** (Fig. 7). GTS generates plots (Fig. 8) showing the relationships among various thermodynamic spaces, including volume versus entropy, pressure versus entropy, volume versus temperature, and pressure versus temperature (that is, the melting curve).

```
(base) zhaoxuan@DESKTOP-QQS359Q:~/GTS/test/MgO/example$ GTS -n MgO -min 40 -max 120

**************************************
  GTS: Gibbs Thermodynamic Surface
       _____   _______    _____
      / ____| |__   __|  / ____|
     | |  __     | |    | (___
     | | |_ |    | |     \___ \
     | |__| |    | |     ____) |
      \_____|    |_|    |_____/
           1.0.4 version
**************************************
        >>>READY TO RUN<<<


--------------------------------------

Obtaining melting points over the specified pressure range...done

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Generating the plot of melting data over the pressure range...done

--------------------------------------
```

Figure 7

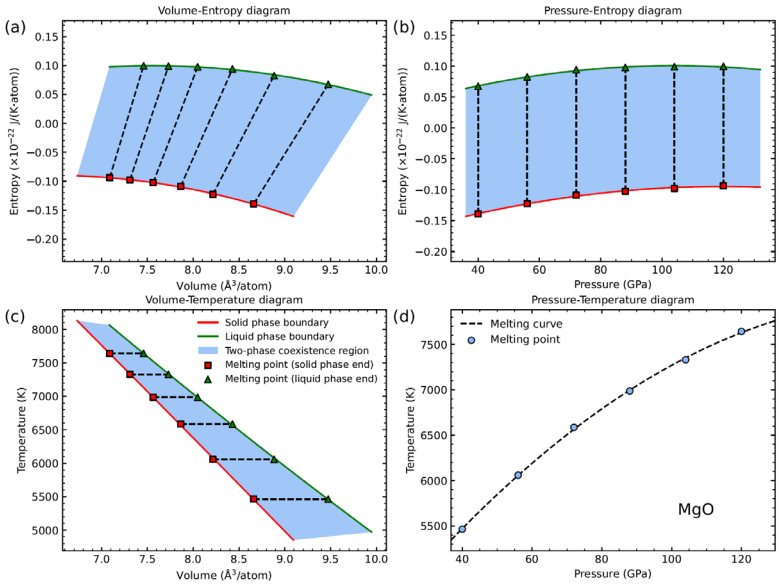

Figure 8

The user can define the step size within the pressure range, execute the command line: **`GTS -n MgO -min 40 -max 120 -num 10`** (Fig. 9&10).

```
(base) zhaoxuan@DESKTOP-QQS359Q:~/GTS/test/MgO/example$ GTS -n MgO -min 40 -max 120 -num 10

************************************
  GTS: Gibbs Thermodynamic Surface
       _____    _______    _____
      / ____|  |__   __|  / ____|
     | |  __      | |    | (___
     | | |_ |     | |     \___ \
     | |__| |     | |     ____) |
      \_____|     |_|    |_____/
           1.0.4 version
************************************
        >>>READY TO RUN<<<


------------------------------------

Obtaining melting points over the specified pressure range...done

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Generating the plot of melting data over the pressure range...done

------------------------------------
```

Figure 9

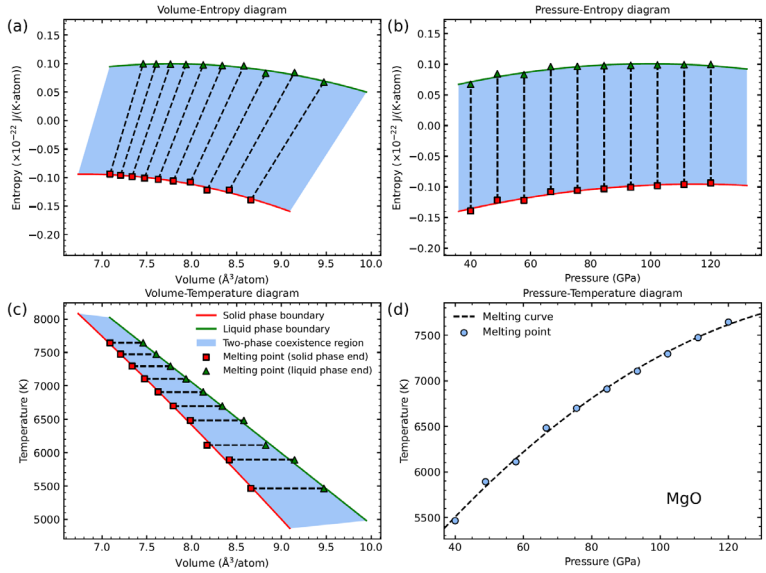

Figure 10

The debug mode for step II. For a single pressure value, GTS will store the fitting data in `MgO_110.0_melting_data` (Fig. 11). For a pressure range, GTS will store the fitting data in `MgO_40.0_120.0_melting_data` (Fig. 12).

```
(base) zhaoxuan@DESKTOP-QQS359Q:~/GTS/test/MgO/example/MgO_110.0_melting_data$ ls -l
total 1740
-rw-r--r-- 1 zhaoxuan zhaoxuan 1717353 Jul  2 17:05 MgO.json
-rw-r--r-- 1 zhaoxuan zhaoxuan   20517 Jul  2 17:05 MgO_pressure_110.000_internal.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   20526 Jul  2 17:05 MgO_pressure_110.000_vasp.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan      40 Jul  2 17:05 cross_point_110.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2285 Jul  2 17:05 liquid_pressure_110.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    1470 Jul  2 17:05 solid_pressure_110.000.txt
```

Figure 11

```
(base) zhaoxuan@DESKTOP-QQS359Q:~/GTS/test/MgO/example/MgO_40.0_120.0_melting_data$ ls -l
total 2056
-rw-r--r-- 1 zhaoxuan zhaoxuan 1717353 Jul  2 17:12 MgO.json
-rw-r--r-- 1 zhaoxuan zhaoxuan   36918 Jul  2 17:12 MgO_40.0_120.0_melting_data.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   20745 Jul  2 17:12 MgO_pressure_104.000_internal.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   20679 Jul  2 17:12 MgO_pressure_104.000_vasp.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   21724 Jul  2 17:12 MgO_pressure_120.000_internal.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   20960 Jul  2 17:12 MgO_pressure_120.000_vasp.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   21454 Jul  2 17:12 MgO_pressure_40.000_internal.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   20690 Jul  2 17:12 MgO_pressure_40.000_vasp.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   21650 Jul  2 17:12 MgO_pressure_56.000_internal.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   20856 Jul  2 17:12 MgO_pressure_56.000_vasp.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   21569 Jul  2 17:12 MgO_pressure_72.000_internal.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   20808 Jul  2 17:12 MgO_pressure_72.000_vasp.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   21816 Jul  2 17:12 MgO_pressure_88.000_internal.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan   20364 Jul  2 17:12 MgO_pressure_88.000_vasp.pdf
-rw-r--r-- 1 zhaoxuan zhaoxuan      98 Jul  2 17:12 cross_point_MgO.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2492 Jul  2 17:12 liquid_pressure_104.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    1936 Jul  2 17:12 liquid_pressure_120.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2516 Jul  2 17:12 liquid_pressure_40.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2889 Jul  2 17:12 liquid_pressure_56.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2564 Jul  2 17:12 liquid_pressure_72.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2520 Jul  2 17:12 liquid_pressure_88.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    1655 Jul  2 17:12 solid_pressure_104.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan     973 Jul  2 17:12 solid_pressure_120.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2552 Jul  2 17:12 solid_pressure_40.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2595 Jul  2 17:12 solid_pressure_56.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2603 Jul  2 17:12 solid_pressure_72.000.txt
-rw-r--r-- 1 zhaoxuan zhaoxuan    2284 Jul  2 17:12 solid_pressure_88.000.txt
```

Figure 12

Requirements

Python version: 3.11.4 or higher

Dependencies: Listed in requirements.txt

Contribution

Contributions are welcome! If you have suggestions or improvements, please feel free to contact us.

License

Contact

Authors:

Kun Yin (yinkun@cdut.edu.cn)

Xuan Zhao