GFNFF Manual

Amsterdam Modeling Suite 2022.1

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CONTENTS

OVERVIEW

The GFN-FF AMS engine is a generic force-field which can be used for elements up to radon (Z=86). It does not require any external force-field file because all parameters are built into the engine.

The main publication for GFN-FF can be found here: Angew. Chemie Int. Edit. 59, 15665-15673 (2020) (https://doi.org/10.1002/anie.202004239).

The version GFN-FF included in AMS is derived from the Jun 29 2021 version of the master branch of https://github.com/grimme-lab/xtb.git.

1.1 Atom typing

Connectivity, atom typing and atomic charges are automatically determined by the GFN-FF engine based on the geometry of the system (if you provide input bonds, they will **not** be used by GFN-FF).

Note: Since connectivity, atom typing and atomic charges are automatically deduced from the geometry, it is important for the input geometry to be "reasonable". If your initial geometry is a heavily distorted molecule, the automatic atom typing procedure might produce unreasonable atom types, which will lead to poor results.

1.2 Parallelization

The current implementation runs on a single processor core only and it should be able to treat systems up to several thousand atoms. For tasks that can take advantage of the AMS driver-level parallelism, you may want to run AMS in parallel.

Tip: The stress tensor is currently calculated numerically with the GFN-FF engine. Therefore you should definitely run in parallel (ideally with `NSCM=12`) for tasks that require its repeated calculated, such as lattice optimizations or MD calculations with a barostat.

1.3 Minimal input

You can set up GFN-FF calculations from AMSInput (see the GUI tutorials for more info) or you can create a run script:

```sh
#!/bin/sh

# Since GFN-FF runs on a single CPU only, here we set
# the number of cores used by AMS to 1.
# For tasks that can take advantage of driver-level
# parallelism, you may want to run AMS in parallel.

export NSCM=1


"$AMSBIN/ams" << eor

Task GeometryOptimization

System
    Atoms
        O 0.0  0.0       0.0
        H 0.0 -0.783836 0.554256
        H 0.0  0.783836 0.554256
    End
End

Engine GFNFF
    # Options for the GFN-FF engine can be specified here.
    # No options are required if you want to use the standard settings.
EndEngine
eor
```

A list of all available input options for GFN-FF can be found *here* (page 3).

KEYWORDS

2.1 Summary of all keywords

`Accuracy`

> **Type** Float
>
> **Default value** 1.0
>
> **Description** Expert option: GFNFF accuracy parameter. Several thresholds within GFNFF depend on this accuracy parameter. Must be a positive number. Smaller values of Accuracy will result in larger distance thresholds.

`ForceFieldFile`

> **Type** String
>
> **Default value**
>
> **GUI name** GFNFF parameter file
>
> **Description** Path to a GFNFF parameter file

`Type`

> **Type** Multiple Choice
>
> **Default value** AngewChem2020_2
>
> **Options** [AngewChem2020, AngewChem2020_1, AngewChem2020_2, FromFile]
>
> **Description** Type of GFNFF to be used

REQUIRED CITATIONS

When you publish results in the scientific literature that were obtained with programs of the AMS package, you are required to include references to the program package with the appropriate release number, and a few key publications.

For calculations using GFN-FF:

S. Spicher, S. Grimme. *Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems*, Angew. Chemie Int. Edit. 59, 15665-15673 (2020) (https://doi.org/10.1002/anie.202004239)