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ufjc: The Python package for the uFJC single-chain model

Michael R. Buche*[1] and Scott J. Grutzik[1]

1 Materials and Failure Modeling, Sandia National Laboratories, Albuquerque, NM 87185, USA

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Software

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Summary

`ufjc` is the Python package that implements the uFJC model for single polymer chains. The uFJC model replaces the rigid links of the freely-jointed chain (FJC) model (Rubinstein & Colby, 2003) with flexible links of potential energy function u (Buche & Silberstein, 2021). This replacement allows the stretching of polymer chains to include bond stretching, and depending on the potential choice, bond breaking (Buche et al., 2022). Through a robust implementation the uFJC single-chain model, the `ufjc` package (1) allows the stretching of polymer chains to be efficiently modeled, (2) is readily integrated into single-chain-based polymer network constitutive models, and (3) provides the tools to study the fundamental statistical thermodynamics of the model system. `ufjc` utilizes efficient capabilities provided by `numpy` (Harris et al., 2020) and `scipy` (Virtanen et al., 2020); visualization using `matplotlib` (Hunter, 2007) is recommended.

Basic usage

The model class is first imported from the package,

```
>>> from ufjc import uFJC
```

and then a model instance may be created,

```
>>> model = uFJC(N_b=8, potential='morse', varepsilon=88)
```

Here, `model` is an instance of the uFJC single-chain model with 8 links, where each link is assigned the Morse (1929) potential with a nondimensional energy scale of 88 (Buche et al., 2022). The model instance has methods corresponding to thermodynamic functions, and results are returned as a `numpy.ndarray`. For example, the nondimensional end-to-end length (extension) of the chain, γ, is computed when a nondimensional force of $\eta = 0.55$ is applied at the ends of the chain:

```
>>> model.gamma(0.55)
array([0.18780929])
```

Other methods include the nondimensional free energy of the chain as a function of extension, the nondimensional probability functions of chain extensions at equilibrium, and the net rate of breaking a chain as a function of extension. Optional keyword arguments in each method are available in order to specify certain features, such as the calculation approach or the thermodynamic ensemble. For example, evaluate the nondimensional equilibrium radial distribution function using the reduced asymptotic approach:

```
>>> model.g_eq([0, 0.23, 0.88], approach='reduced')
array([0.00000000e+00, 2.64707367e+00, 1.24115933e-04])
```

These functions are plotted over an exemplary range of parameters in Figure 1.

*mrbuche@sandia.gov

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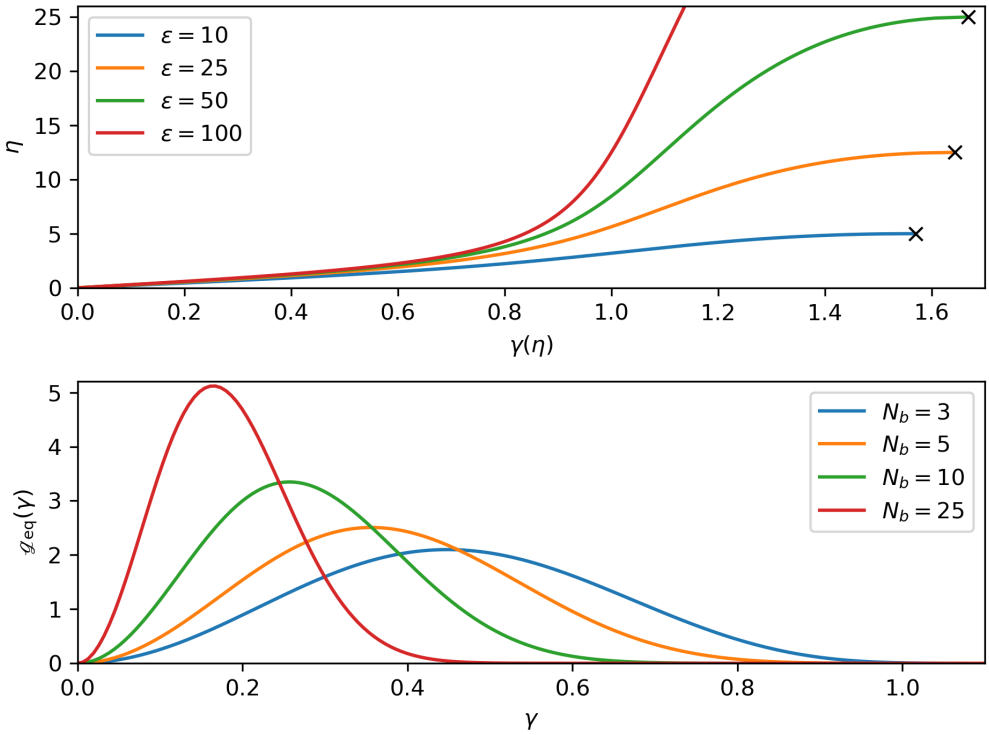

Figure 1: Thermodynamic functions for the Morse-FJC model with base parameters $N_b = 8$, $\alpha = 1$, and $\varepsilon = 88$. (top) The nondimensional single-chain mechanical response (force versus extension) for an increasing nondimensional potential energy scale. An x denotes the maximum force that the chain can sustain, where additional force would cause breaking. (bottom) The nondimensional equilibrium radial distribution function versus extension for an increasing number of links.

Statement of need

`ufjc` was developed for researchers to effectively model single polymer chains and networks of polymer chains. Researchers have historically relied on the freely-jointed chain (FJC) model, which captures fundamental physics while maintaining analytic simplicity. The FJC model consists of a number of rigid phantom links connected in series by penalty-free hinges; the increasing force required to extend the chain is due to entropy reduction, and is described by the Langevin function (Rubinstein & Colby, 2003). Researchers have become interested in modeling polymers up to and including failure, but unfortunately the rigid links of the FJC model are neither capable of modeling bond stretching nor breaking. The rigid links can be made flexible according to some potential energy function u, but this causes the model to become analytically intractable, except for the special case of a harmonic potential and the isotensional ensemble (Balabaev & Khazanovich, 2009; Buche & Silberstein, 2020; Manca et al., 2012). Quite recently, an asymptotically-correct statistical thermodynamic theory (Buche, 2021) has been successfully applied to this uFJC model, resulting in accurate, analytically-tractable relations for the model for steep link potentials (Buche et al., 2022). The `ufjc` package robustly implements this approach, enabling the results presented by Buche et al. (2022) while providing many additional functionalities. The object-oriented structure of `ufjc` allows it to be readily integrated into other packages as a sub-package, such as polymer network constitutive models that build up from a single-chain models. Correspondingly, `ufjc` will streamline ongoing constitutive model development, and improve existing constitutive models through reimplementation (Buche & Silberstein, 2021).

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