Setting up ESPResSo for FFS sampling with FRESHS

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1 Introduction

Welcome to the forward flux sampling (FFS) **ESPResSo** tutorial!

This tutorial assumes basic **ESPResSo** and FFS knowledge. We will use the software package **FRESHS** which so far has three rare event sampling techniques implemented, namely SPRES, FFS and PERMFFS. We will focus on the direct FFS method (sometimes called dFFS in the literature) to drive a system through a transition. General instructions for arbitrary rare event systems will be accompanied by a model system of unbiased polymertranslocation. First we will discuss how to setup the **FRESHS** server and client configurations, as shown in Sec. 2.

2 FRESHS Setup

3 Changes to your simulation script

4 Running your simulation

5 Obtaining transition rates and interface statistics