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GaPFlow: Gap-averaged flow simulations with Gaussian process regression

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Summary

Fluid flow in confined geometries is common in both natural systems and many engineering applications. When the characteristic length of the confining dimension approaches the nanometer scale, the molecular nature of the fluid can no longer be neglected. This is particularly relevant for lubricated frictional contacts, where surface roughness can lead to local gap heights of only a few nanometers (Archard et al., 1962; Glovnea et al., 2003). The constitutive laws that describe the fluid's response to extreme loading conditions (e.g. high shear rates) need to account for molecular effects, such as shear thinning (Jadhao & Robbins, 2019), fluid layering (Gao et al., 1997), or wall slip (Pit et al., 2000; Zhu & Granick, 2001).

Molecular dynamics (MD) simulations have become a standard tool to provide insights into these nanoscale phenomena (Ewen et al., 2018), but their direct use in macroscopic simulations is challenging. GaPFlow addresses this gap by enabling concurrent multiscale simulations of nanofluidic flows, in which MD data are incorporated on demand through nonparametric surrogate models based on probabilistic machine learning. This approach allows the simulation to adapt to previously unseen local flow conditions and provides uncertainty estimates for predicted shear and normal stresses in lubricated contacts.

Statement of need

`GaPFlow` is a numerical solver for fluid flows in confined geometries, such as the narrow gaps found in lubricated contacts. Traditional lubrication models solve the Reynolds equation (Reynolds, 1886), a simplified form of the Navier-Stokes equation expressed as a single partial differential equation for the fluid pressure. MD simulations have been used to parameterize common constitutive laws for viscosity and wall slip (Codrignani et al., 2023; Martini et al., 2006; Savio et al., 2015), which can be readily incorporated into existing lubrication solvers. However, they lack the feedback mechanism from the macroscopic to the molecular scale. The rigidity of purely sequential coupling schemes suggests that they are not ideal for capturing the extreme and diverse environments typical for frictional contacts.

In contrast, `GaPFlow` solves the lubrication problem in the formulation proposed by Holey et al. (2022), which evolves gap-averaged conserved quantities, such as mass or momentum, in time. This formulation is agnostic to the constitutive behavior of the confined fluid, making it suitable for multiscale simulations in which the fluid response is provided by molecular dynamics (MD) simulations. `GaPFlow` uses a surrogate model based on Gaussian process (GP) regression to interpolate between data obtained from MD, and to select new configurations based on the GP uncertainty to augment an existing MD database (a.k.a. active learning) (Holey et al., 2025). Earlier versions of `GaPFlow` have been used in three publications so far (Holey et al., 2022; Holey et al., 2024, 2025).

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Components and external dependencies

GaPFlow's core functionality is the numerical solution of the gap-averaged balance equations as introduced by Holey et al. (2022) for lubrication problems. Averaging the general form of a conservation law over the gap coordinate (z) with spatially and temporally varying integral bounds, i.e. the topographies of the lower (h_0) and upper wall (h_1), leads to a balance law of the form

$$\frac{\partial \bar{\mathbf{q}}}{\partial t} = -\frac{\partial \bar{\mathbf{f}}_x}{\partial x} - \frac{\partial \bar{\mathbf{f}}_y}{\partial y} - \mathbf{s},$$

where $\bar{\mathbf{q}} \equiv \bar{\mathbf{q}}(x,y,t) = h^{-1}\int_{h_0}^{h_1} \mathbf{q}(x,y,z,t)dz$ collects the densities of conserved variables (e.g. $\mathbf{q} = (\rho, j_x, j_y)^\top$ for mass and in-plane momentum) and $\bar{\mathbf{f}}_i \equiv \bar{\mathbf{f}}_i(x,y,t) = h^{-1}\int_{h_0}^{h_1} \mathbf{f}_i(x,y,z,t)dz$ are the corresponding fluxes in direction $i \in \{x,y\}$ with $h = h_1 - h_0$. The source term $\mathbf{s}$ accounts for fluxes across the bottom and top walls ($\mathbf{f}_z$) as well as for changes in the conserved variable densities induced by flow within a spatially varying gap. The current implementation uses a finite volume discretization on a regular grid and the MacCormack explicit time-integration scheme (MacCormack, 2003) to solve the transient lubrication problem. The µGrid library is used to assemble the discretized density and flux fields into a unified container and to export the simulation results in the NetCDF file format.

Next to the numerical inegration of the continuum equations, GaPFlow serves as a *glue code* that integrates the various components for multiscale or multiphysics simulations. Therefore, it relies on a small set of external dependencies which are summarized below.

GP regression

The fluxes required to close the macroscopic equations can either be obtained from deterministic constitutive laws or modeled using GP regression (Rasmussen & Williams, 2006). The GP models are trained on data generated by MD, or, for testing purposes, on sparsified datasets sampled from predefined constitutive laws. GaPFlow employs the tinygp library for constructing and training GP models, taking advantage of its flexibility. For example, it allows the implementation of custom kernels for the joint prediction of wall shear stresses at the top and bottom walls using a multi-output GP that shares a common noise process. Since tinygp is built on JAX, GaPFlow also benefits from automatic differentiation of the GP models, e.g. to compute the speed of sound from the pressure model.

Automatic setup of MD runs

In active learning simulations the GP uncertainty determines when and where new MD data are required. When this occurs, the main simulation loop pauses and waits for the MD simulation to complete. GaPFlow uses the Python interface of LAMMPS (Thompson et al., 2022) to execute these simulations in parallel. The correct and fully automated setup of MD runs is likely the most critical step in the multiscale framework. To facilitate this process, users can subclass the abstract base class `GaPFlow.md.MolecularDynamics` implementing only two methods: one for generating the input files and one for reading the output files. This design gives users complete control over the MD setup while maintaining a consistent interface with the main solver. GaPFlow provides two examples how this can be done: 1. A simple example that relies entirely on LAMMPS to set up a Lennard-Jones system (fluid and walls), and 2. A more advanced example that uses ASE (Larsen et al., 2017) and moltemplate (Jewett et al., 2021) to construct an alkane fluid confined between gold walls. Both MD setups use the Gaussian dynamics algorithm by Strong & Eaves (2017) to control the mass flux according to the continuum solution, as implemented in LAMMPS.

Data management

Running MD simulations is the computationally most expensive component of the multiscale framework. Although the active learning scheme ensures that the database grows only as needed, it is desirable to re-use this database across future simulations. Achieving this requires a dedicated data management strategy, ideally following the FAIR principles (Wilkinson et al., 2016). `GaPFlow` uses `dtool` (Olsson & Hartley, 2019) to package the inputs and outputs of individual MD runs into immutable datasets with unique persistent identifiers, together with automatically generated metadata. Users can operate on these datasets locally, but `GaPFlow` can also be readily integrated with a `dserver` instance (Hörmann et al., 2024), which indexes the metadata stored on a remote device. This makes it straightforward to discover previously computed configurations, or to share datasets with collaborators.

Elastic deformations

In non-conforming lubricated contacts such as in ball or roller bearings, local fluid pressures can become large such that elastic deformation of the walls can no longer be neglected. For simulations in this *Elastohydrodynamic Regime*, `GaPFlow` uses the ContactMechanics code which is part of the contact.engineering (Röttger et al., 2022) ecosystem to compute elastic deformations of the walls in contact with the fluid. Under the assumption that the elastic deformation of the walls responds on a timescale much shorter than that of the fluid-dynamic system, the elastic response can be treated as quasi-static and represented by its steady-state solution. Further assuming linear-elastic and isotropic walls, the tool utilizes a *Green's function* formulation that reduces the computational effort to a convolution operation, which can be efficiently solved in Fourier space (Stanley & Kato, 1997). The elastic deformation is determined based on the fluid pressure field and automatically adapts to the boundary conditions specified in the fluid-flow problem. Fluid flow and wall deformation are linked through a *weak coupling* scheme in which both solutions are iteratively updated,.

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