Mango-Selm Software: Fluid-Structure Interaction subject to Thermal Fluctuations
Soft Materials, Biophysics, Fluidics

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Mango-Selm Software: Overview

**Selm - Simulation Package:**

SELM fluctuating hydrodynamics for fluid-structure interactions subject to thermal fluctuations.

- Python, Jupyter notebooks, and other scripting for model building and simulation.
- Stochastic numerical time-step integrators for inertial and quasi-steady physical regimes in (C/C++)

**Molecular dynamics integration with LAMMPS**

- Modeling, interactions, many potentials, statistical analysis.
- Thermostats and many ensembles possible such as Lees-Edwards for shear simulations.

**Standardized formats**

- XML for parametrization and data output.
- VTK output for continuum fields and microstructures (visualization / analysis).

**Mango – GUI for Model Building:**

Graphical User Interface (GUI) for setting up model geometry and simulation parameters.

- Generates scripts and data files for SELM fluctuating hydrodynamics simulations.

**Extendible object-oriented architectures** for inclusion of new numerical methods.

Motivations

Stochastic Immersed Boundary Methods (SIBMs)
Eulerian-Lagrangian Methods (ELMs)
Implicit-Solvent Coarse-Grained (IS-CG) Simulations
**Soft Materials / Complex Fluids**
- Microstructure interactions on the order of $k_B T$.
- Properties arise from balance of entropy-enthalpy.
- Solvent plays important role (interactions / dynamic responses).

**Approaches**
- Atomistic Molecular Dynamics.
- Continuum Mechanics.
- Coarse-Grained Particle Models (solvated or implicitly treated).
- Challenges from phenomena spanning wide temporal-spatial scales.

**Simulation Aims**
- Investigate how larger-scale mechanics arise from microstructure interactions / kinetics.
- Capture roles of solvent mediated interactions efficiently (i.e. continuum level).
- Resolve microstructure mechanics and dynamics.
- Computational efficiencies allow for accessing larger length and time-scales for investigating wider class of phenomena.
Fluctuations arise from spontaneous momentum transfer from molecular-level collisions.

Stochastic model of thermal fluctuations captured through random stress $\Sigma \sim$ Gaussian.

Challenges for analysis and numerical methods presented from the $\delta$-correlation in space-time.

Fluid-structure interactions: How to incorporate tractably?
Stochastic Eulerian Lagrangian Methods (SELMs) for Fluid-Structure Interactions

**Fluid Equations**

\[
\begin{align*}
\rho \frac{\partial \mathbf{u}}{\partial t} &= \mathcal{L} \mathbf{u} + \Lambda [\mathcal{Y} (\mathbf{v} - \Gamma \mathbf{u})] + \lambda + \mathbf{f}_{\text{thm}} \\
\nabla \cdot \mathbf{u} &= 0
\end{align*}
\]

**Microstructure Equations**

\[
\begin{align*}
\frac{d \mathbf{X}}{dt} &= \mathbf{v} \\
m \frac{d \mathbf{v}}{dt} &= -\mathcal{Y} (\mathbf{v} - \Gamma \mathbf{u}) - \nabla \mathbf{X} \Phi [\mathbf{X}] + \zeta + \mathbf{F}_{\text{thm}}
\end{align*}
\]

**Thermal Fluctuations**

\[
\begin{align*}
\langle \mathbf{f}_{\text{thm}} (s) \mathbf{f}_{\text{thm}}^T (t) \rangle &= - (2k_B T) (\mathcal{L} - \Lambda \mathcal{Y} \Gamma) \delta (t - s) \\
\langle \mathbf{F}_{\text{thm}} (s) \mathbf{F}_{\text{thm}}^T (t) \rangle &= (2k_B T) \mathcal{Y} \delta (t - s) \\
\langle \mathbf{f}_{\text{thm}} (s) \mathbf{F}_{\text{thm}}^T (t) \rangle &= - (2k_B T) \Lambda \mathcal{Y} \delta (t - s)
\end{align*}
\]

**Operators:**

- \(\mathcal{L}\) → Fluid dissipation (viscosity).
- \(\mathcal{Y}\) → Structure “slip” relative to local flow field.
- \(\Gamma\) → Kinematic particle velocity for given flow.
- \(\Lambda\) → Induced fluid force density from particle.

**Notation:**

- \(\mathbf{u} = \mathbf{u}(\mathbf{x}, t)\) → Fluid velocity.
- \(\mathbf{X} = \mathbf{X}(\mathbf{q}, t)\) → Structure configuration.
- \(\mathbf{v} = \mathbf{v}(\mathbf{q}, t)\) → Structure velocity.
**Thermostats**

**Berendson, Nose-Hoover**

\[ \frac{dV}{dt} = -\gamma V - \nabla \Phi(X) + \sqrt{2k_B T\gamma} \frac{dB_t}{dt} \]

\[ \frac{dX}{dt} = V. \]

missing correlations through solvent!

**Langevin**

\[ \frac{dV}{dt} = -\gamma V - \nabla \Phi(X) + \sqrt{2k_B T\gamma} \frac{dB_t}{dt} \]

\[ \frac{dX}{dt} = V. \]

**Fluctuating Hydrodynamics**

\[ \frac{dX}{dt} = \nu \]

\[ m\frac{d\nu}{dt} = -\gamma (\nu - \Gamma u) - \nabla X \Phi[X] + \zeta + F_{\text{thm}} \]

lateral momentum transfer: correlations
Coupling Operators, Immersed Boundary Methods

SELM Coupling:

adjoint condition

\[ \langle \Gamma v_\gamma F \rangle = \sum_i \frac{\partial}{\partial v_i} \cdot F_i = \int_{\Omega} v(x) \cdot (\Lambda F)(x) \, dx = \langle v, \Lambda F \rangle \]

IB-Kernel coupling:

\[ \Gamma u = \int_{\Omega} \eta (y - X(t)) u(y, t) \, dy \]
\[ \Lambda F = \eta (x - X(t)) F. \]

Generalized Coupling (Faxen)

\[ \Gamma_0 u = \sum_m \langle \eta_0 (y_m - (X_{cm} + z)) \cdot u_m \rangle_{S,|x|=R} \Delta x_m^3 \]
\[ \Gamma_1 u = \frac{3}{2R^2} \sum_m \langle \eta_1 (y_m - (X_{cm} + z)) (z \times u_m) \rangle_{S,|x|=R} \Delta x_m^3. \]
\[ \Lambda_0 (x_m) = \left( \frac{\eta_0 (x_m - (X_{cm} + z))}{S,|x|=R} \right) F \]
\[ \Lambda_1 (x_m) = -\frac{3}{2R^2} \left( \langle z \eta_1 (x_m - (X_{cm} + z)) \rangle_{S,|x|=R} \right) \times T. \]
### Summary of Regimes for SELMs

#### Stochastic Eulerian Lagrangian Methods (SELMs)

**Fluid dynamics:**
\[
\begin{align*}
  \frac{\partial u}{\partial t} &= \mu \Delta u - \nabla p + \Lambda \left[ (v - \Gamma u) \right] + f_{\text{thm}} \\
  \nabla \cdot u &= 0
\end{align*}
\]

**Structure dynamics:**
\[
\begin{align*}
  \frac{dX}{dt} &= v \\
  m \frac{d\nu}{dt} &= -\Upsilon (v - \Gamma u) - \nabla_x \Phi[X] + \zeta + F_{\text{thm}}
\end{align*}
\]

**Thermal Fluctuations:**
\[
\begin{align*}
  \langle f_{\text{thm}}(s)F^T_{\text{thm}}(t) \rangle &= -(2k_B T) \mu \Delta \Lambda \Upsilon \delta(t-s) \\
  \langle F_{\text{thm}}(s)F^T_{\text{thm}}(t) \rangle &= (2k_B T) \Upsilon \delta(t-s) \\
  \langle f_{\text{thm}}(s)F^T_{\text{thm}}(t) \rangle &= -(2k_B T) \Lambda \Upsilon \delta(t-s).
\end{align*}
\]

#### Fluid-structure equations: Microstructure-fluid no-slip coupling (S-Immersed-Boundary)

**Structure momentum no longer tracked.**
- Removes a source of stiffness.
- Non-conjugate Hamiltonian formulation yields metric-factor in phase-space.

#### Microstructure density matched with fluid

**Fluid-structure dynamics:**
\[
\begin{align*}
  \frac{dp}{dt} &= \rho^{-1} \Gamma p + \Lambda \left[ -\nabla_x \Phi(X) \right] - \left( \nabla_x \cdot \Lambda \right) k_B T + \lambda + g_{\text{thm}} \\
  \frac{dX}{dt} &= \rho^{-1} \Gamma p
\end{align*}
\]

**Thermal Fluctuations:**
\[
\begin{align*}
  \langle g_{\text{thm}}(s)g^T_{\text{thm}}(t) \rangle &= -(2k_B T) \zeta \delta(t-s) \\
  \langle G_{\text{thm}}(s)G^T_{\text{thm}}(t) \rangle &= (2k_B T) \zeta T^{-1} \delta(t-s) \\
  \langle g_{\text{thm}}(s)G^T_{\text{thm}}(t) \rangle &= 0.
\end{align*}
\]

- Structure momentum no longer tracked.
- Removes a source of stiffness.
- Non-conjugate Hamiltonian formulation yields metric-factor in phase-space.

#### Fluid-structure equations: Microstructure-fluid stress balance

**Structure momentum no longer tracked.**
- Balance of hydrodynamic stresses with elastic stresses.
- Removes additional sources of stiffness.
- Phase-space metric reflected in the drift term.
SELM-LAMMPS Integration

Molecular Dynamics and Coarse-Grained Modeling Approaches
Mango-Selm Software: Overview

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Mango – GUI for Model Building:
Graphical User Interface (GUI) for setting up model geometry and simulation parameters.
  - Generates scripts and data files for SELM fluctuating hydrodynamics simulations.

Extendible object-oriented architectures for inclusion of new numerical methods.

Download: http://mango-selm.org/
Mango-Selm Implementation
SELMS − Source Codes:

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Features:

- **Object-oriented C++ classes** mirroring parts of SELM with XML parameter files.
- **Delegator design pattern** is used to control the work-flow.
- **Four main SELM classes** correspond to:
  - Eulerian Mechanics
  - Lagrangian Mechanics
  - Fluid-Structure Coupling (Eulerian-Lagrangian communication)
  - Time-Step Integration
- **Additional classes** for XML parsing, data generation.
- **Designed to be easily extended** for new types of SELM formulations and integrators.
Mango GUI Model Builder

Mango - Modeling Software:

Mango Model Builder for Stochastic Eulerian Lagrangian Methods
Version 2.1.1
Paul J. Atzberger

Python Interactive Editor 1.0: Implemented by Paul J. Atzberger, copyright 2013.

Startup Script for MAM Python Interpreter
Written by Paul J. Atzberger
Date: March, 2011.

Model Build Package 1: Authored by Paul J. Atzberger; Version 1.0
Setup appears to have completed with no known errors.

Atzberger 2016
Mango Modeling Software

Mango - Codes

Atzberger 2016

Paul J. Atzberger

http://atzberger.org/

UC Santa Barbara
Mango Modeling Software

MANGO - Codes

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<td>Atz_Struct_DataChangeListener_MainData.java</td>
<td>JTable Preferences_TableDisplay.java</td>
</tr>
</tbody>
</table>

Features:

- **Object-oriented classes in Java** mirroring parts of SELM.
- **Dynamic object loaders** for delegator design pattern for control flow (extension after compiled byte-codes).
- **Four main SELM classes** correspond to:
  - Eulerian Mechanics
  - Lagrangian Mechanics
  - Fluid-Structure Coupling (Eulerian-Lagrangian communication)
  - Time-Step Integration
- **Designed to be easily extended** for new types of SELM formulations and integrators.
- **Custom classes and interfaces** for rendering models in 3D and interactively editing models.

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Mango Modeling Software

Mango – Codes:

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<td>Atz_UnitsRef.java</td>
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Custom classes implemented for tracking physical units in tables.
Mango GUI Jython Interface

MANGO - Modeling Software:

Custom classes implement interactive terminal based on Jython.
Wrapper jython classes implemented for MANGO interface and SELM data structures.
Editor features allow for
- jython/python scripting to construct models
- custom GUI windows : interactive components in MANGO
- post-processing scripts
- generation of SELM XML files from the constructed MANGO data structures.

Jupyter notebooks and Python interface now also available (directly with Selm-Lammps library).

Python and Jupyter notebook interfaces

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Selm-Lammps Integration

Python and Jupyter Notebook Interfaces
Tips for SELM Package: Installation and Usage

Instructions

Download at: http://mango-selm.org/

Installation in Linux preferred: Ubuntu 18.04 or 20.04 (pre-compiled binaries available).

Directories:
- /bin: collection of pre-compiled binaries.
- SELM-LAMMPS/src/USER-SELM: main C/C++ codes for SELM package
- SELM-LAMMPS/src/USER-SELM/examples: example models and simulation scripts

Installing Python components (uses lammps.py, lammps.so):
- Conda or virtualenv determine dir by “which python”
- Copy shared library and files into XX/site-packages/ directory.
- Create symbolic links to the shared library and binaries (or put in path)
  - ln –s XXX/bin/lammps.so lammps.so
- See examples directory for Jupyter notebooks, python scripts, for running simulations.
- See README files for more details.

Jupyter Notebooks and Python-based Simulations:
- Uses python-interfaces to LAMMPs.
- L.command(cmd_str); runs the command in cmd_str.
- Model building using python wrapper
  - sets up particles
  - sets up interactions, many possible types and potential available
  - sets up the simulation parameters.
Create Selm-Lammps instance

Setup the Simulation Files (such as .read_data)

In [125]:
    
    num_dim = 2
    num_part = 1
    num_atm = 5
    num_mol = 10

    # setup box
    box = np.linspace(num_part, num_part, num_mol) + np.linspace(0., 1.0, num_mol)

    # setup particles
    x1 = 0.
    y1 = 0.

    # setup interactions
    kappa = [0.1, 0.2, 0.3, 0.4, 0.5]

    # setup model
    mol_info = np.random.randint(0, 5, size=(num_mol, 1))

    # setup code
    code = ['(x1, y1)', 'x1, y1]

Model configuration (generated file)

Set up the interaction parameters

Setup parameters

SEL: LAMMPS XML file

Running simulation and analysis

Interface allows for:
- checking intermediate results
- resuming simulations
- performing analysis and visualization.
How to Setup Model in Practice

Example
Polymer: Thermal Fluctuations with Hydrodynamic Correlations

Directory:
/SELM-LAMMPS/src/USER-SELM/examples/Polymer4

Jupyter notebook:
simulation_polymer4.ipynb

Create Selm-Lammps instance

Setup model geometry and interactions

Run simulation and analysis

SELM XML files
Conclusions

Summary

**Stochastic Immersed Boundary Methods** with numerical solvers preserving statistical mechanics properties.

**Stochastic Eulerian Lagrangian Methods** for inertial and overdamped regimes, various boundary conditions.

**Python interface** for setting up simulations, **LAMMPS molecular dynamics integration** (modeling, analysis).

**Applications** in soft materials, complex fluids, rheology, microfluidics, biophysics, lipid bilayer membranes.

Papers


UCSB Recent Student Collaborators


Sandia Collaborators

N. Trask, P. Kuberry, J. Hu, C. Siefert, and others.

Funding

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