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

April 2021

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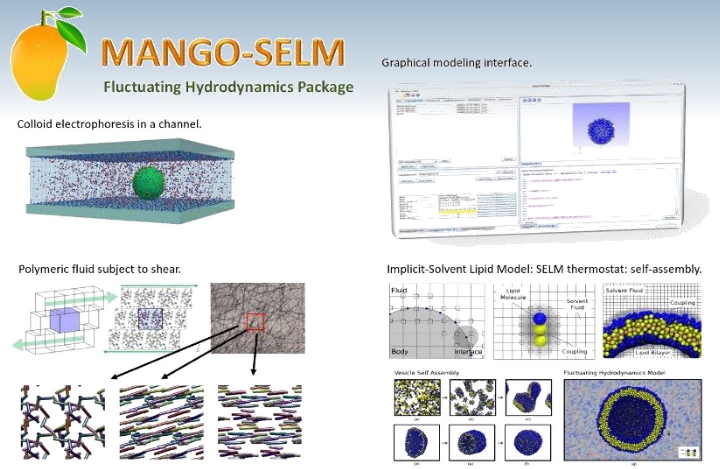
DOE ASCR CM4
DE-SC0009254

DOE ASCR PhILMS
DE-SC0019246

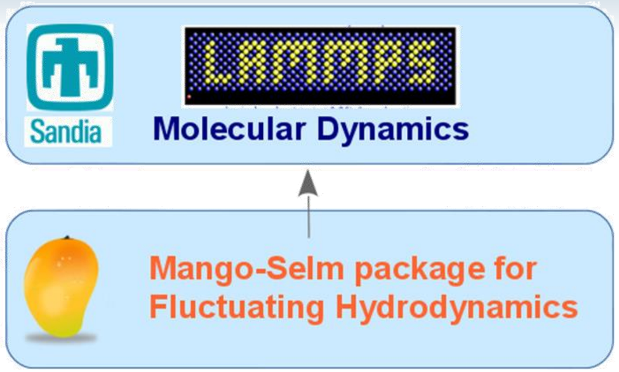
NSF Grant
DMS - 1616353

NSF CAREER Grant
DMS-0956210

Mango-Selm Software: Overview



Molecular dynamics Integration



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

Python and Jupyter notebook interfaces

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).

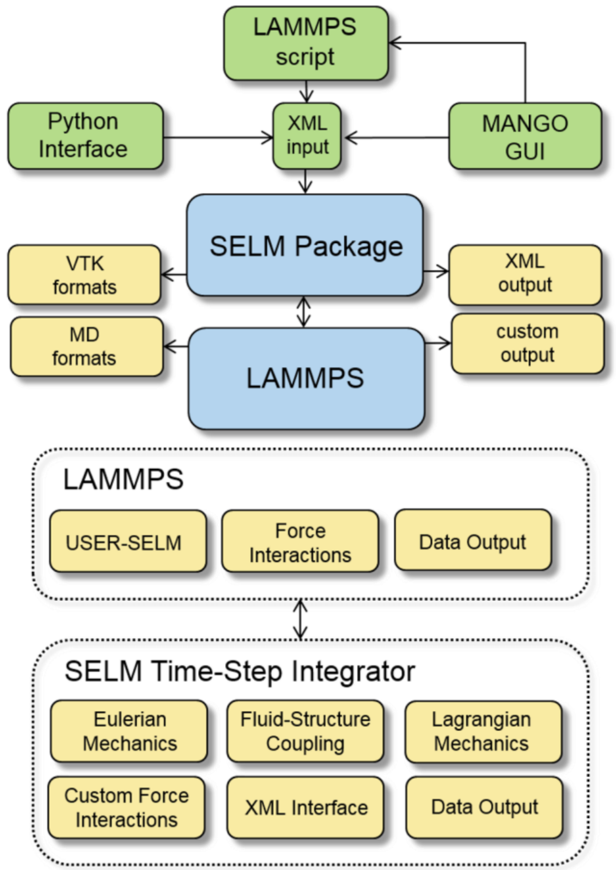
Mango – GUI for Model Building:

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.

Modular Design and Extendible

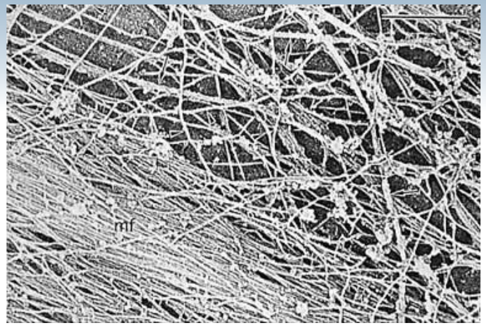


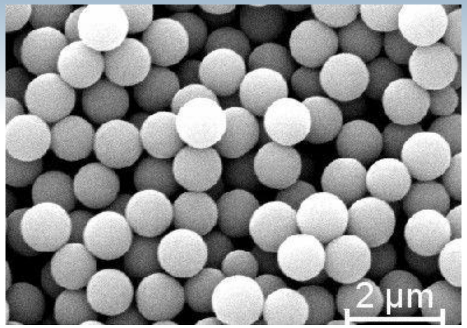
Atzberger 2016

Motivations

Stochastic Immersed Boundary Methods (SIBMs)
Eulerian-Lagrangian Methods (ELMs)
Implicit-Solvent Coarse-Grained (IS-CG) Simulations

Motivations: Soft Materials, Complex Fluids, and Other Applications


Gels (Actin)

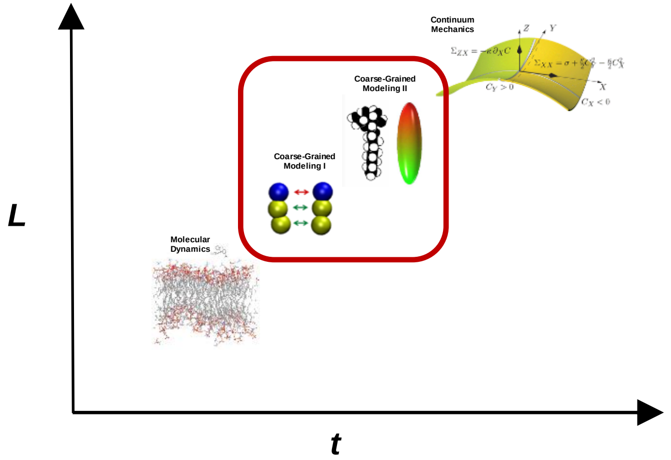


Colloids


Membranes (lipids)

Soft Materials / Complex Fluids

- Microstructure interactions on the order of K_BT.
- Properties arise from balance of entropy-enthalpy.
- Solvent plays important role (interactions / dynamic responses).

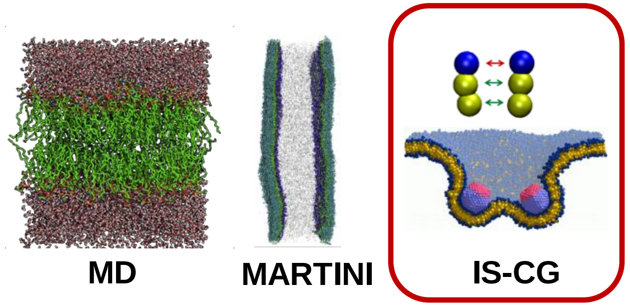


Approaches

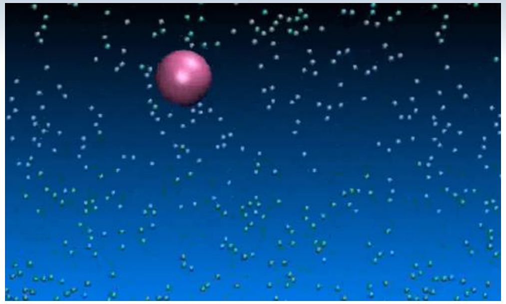
- Atomistic Molecular Dynamics.
- Continuum Mechanics.
- Coarse-Grained Particle Models (solvated or implicitly treated).
- Challenges from phenomena spanning wide temporal-spatial scales.

Simulation Aims

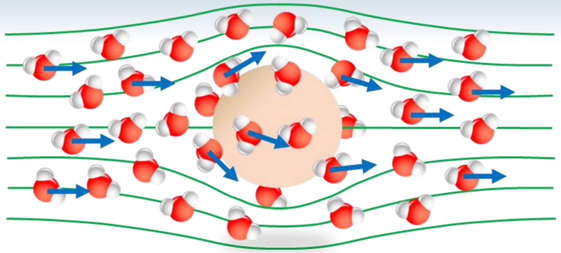
- Investigate how larger-scale mechanics arise from microstructure interactions / kinetics.
- Capture roles of solvent mediated interactions efficiently (i.e. continuum level).
- Resolve microstructure mechanics and dynamics.
- Computational efficiencies allow for accessing larger length and time-scales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



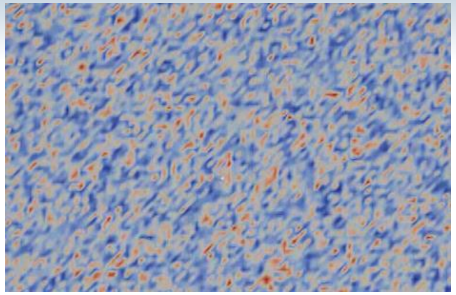
Fluctuating Hydrodynamics



Brownian Motion: Molecular Collisions



Hydrodynamics + Fluctuations



Continuum Gaussian Random Field

Landau-Lifschitz fluctuating hydrodynamics

$$\rho\left(\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + \mathbf{u}(\mathbf{x},t)\cdot\nabla\mathbf{u}(\mathbf{x},t)\right) = \mu\Delta\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \nabla\cdot\mathbf{\Sigma}(\mathbf{x},t).$$

$$\nabla\cdot\mathbf{u}(\mathbf{x},t) = 0.$$

$$\langle \Sigma_{ij}(\mathbf{x},t)\Sigma_{kl}(\mathbf{y},s)\rangle = 2\mu k_B T\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\delta(\mathbf{x}-\mathbf{y})\delta(t-s).$$

Fluctuations arise from spontaneous momentum transfer from molecular-level collisions.

Stochastic model of thermal fluctuations captured through random stress Σ ~ Gaussian.

Challenges for analysis and numerical methods presented from the δ-correlation in space-time.

Fluid-structure interactions: How to incorporate tractably?

Stochastic Eulerian Lagrangian Methods (SELMs) for Fluid-Structure Interactions

Fluid Equations

$$\rho \frac{\partial \mathbf{u}}{\partial t} = \mathcal{L}\mathbf{u} + \Lambda[\Upsilon(\mathbf{v} - \Gamma\mathbf{u})] + \lambda + \mathbf{f}_{\mathrm{thm}}$$
$$\nabla \cdot \mathbf{u} = 0$$

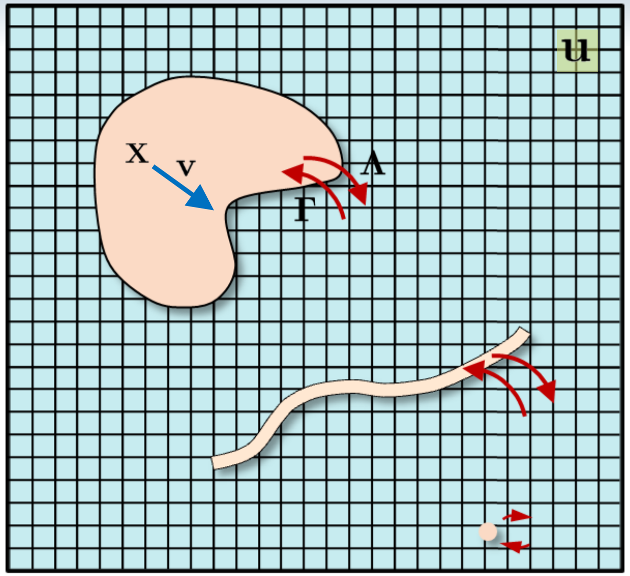
Microstructure Equations

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}$$
$$m\frac{d\mathbf{v}}{dt} = -\Upsilon\left(\mathbf{v} - \Gamma\mathbf{u}\right) - \nabla_{\mathbf{X}}\Phi[\mathbf{X}] + \zeta + \mathbf{F}_{\mathrm{thm}}$$

Thermal Fluctuations

$$\langle \mathbf{f}_{\mathrm{thm}}(s)\mathbf{f}_{\mathrm{thm}}^T(t)\rangle = -\left(2k_BT\right)\left(\mathcal{L} - \Lambda\Upsilon\Gamma\right)\delta(t-s)$$
$$\langle \mathbf{F}_{\mathrm{thm}}(s)\mathbf{F}_{\mathrm{thm}}^T(t)\rangle = \left(2k_BT\right)\Upsilon\,\delta(t-s)$$
$$\langle \mathbf{f}_{\mathrm{thm}}(s)\mathbf{F}_{\mathrm{thm}}^T(t)\rangle = -\left(2k_BT\right)\Lambda\Upsilon\,\delta(t-s).$$

Eulerian-Lagrangian Approach



Operators:

$\mathcal{L} \longrightarrow$ Fluid dissipation (viscosity).

$\Upsilon \longrightarrow$ Structure "slip" relative to local flow field.

$\Gamma \longrightarrow$ Kinematic particle velocity for given flow.

$\Lambda \longrightarrow$ Induced fluid force density from particle.

Notation:

$\mathbf{u} = \mathbf{u}(\mathbf{x}, t) \longrightarrow$ Fluid velocity.

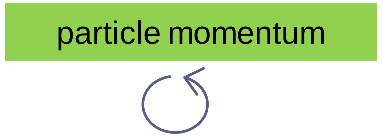
$\mathbf{X} = \mathbf{X}(\mathbf{q}, t) \longrightarrow$ Structure configuration

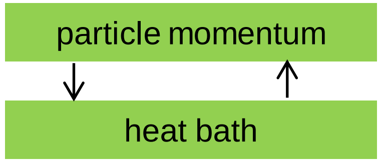
$\mathbf{v} = \mathbf{v}(\mathbf{q}, t) \longrightarrow$ Structure velocity.

Peskin, Kramer, Atzberger 2007, Atzberger 2011

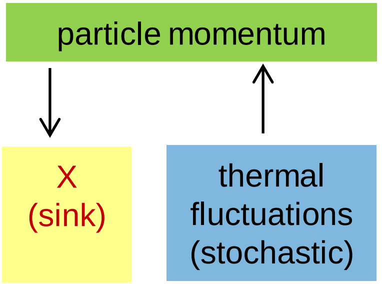
Thermostats

Berendson, Nose-Hoover





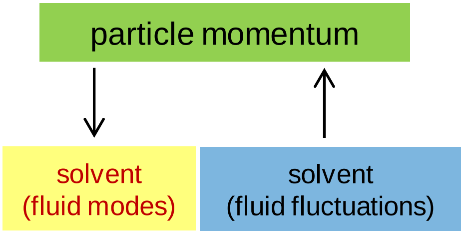
Langevin



$$
\begin{aligned}
m\frac{d\mathbf{V}}{dt} &= -\gamma\mathbf{V} - \nabla\Phi(\mathbf{X}) + \sqrt{2k_BT\gamma}\,\frac{d\mathbf{B}_t}{dt} \\
\frac{d\mathbf{X}}{dt} &= \mathbf{V}.
\end{aligned}
$$

missing correlations through solvent!

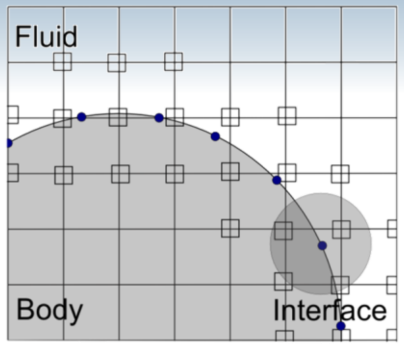
Fluctuating Hydrodynamics

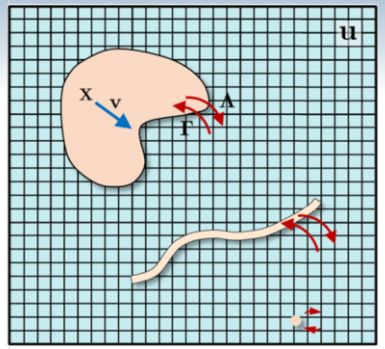


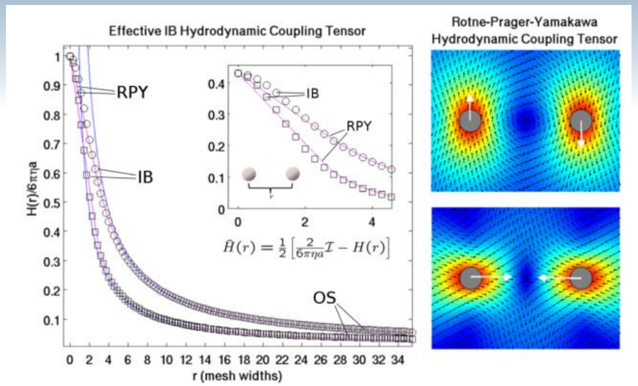
$$
\begin{aligned}
\frac{d\mathbf{X}}{dt} &= \mathbf{v} \\
m\frac{d\mathbf{v}}{dt} &= -\Upsilon\left(\mathbf{v} - \Gamma\mathbf{u}\right) - \nabla_{\mathbf{X}}\Phi[\mathbf{X}] + \zeta + \mathbf{F}_{\mathrm{thm}}
\end{aligned}
$$

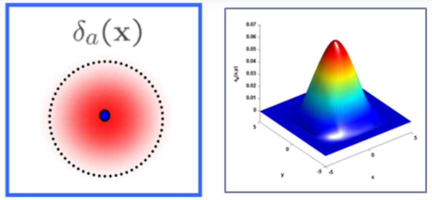
lateral momentum transfer : correlations

Coupling Operators, Immersed Boundary Methods









Peskin delta-function

SELM Coupling:

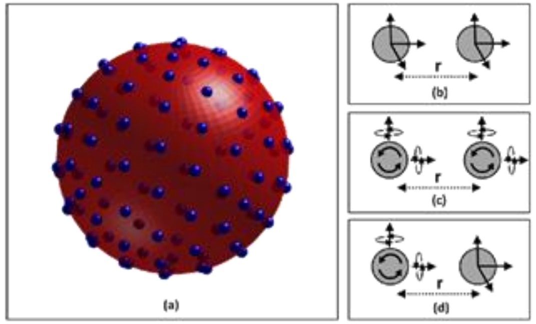
adjoint condition

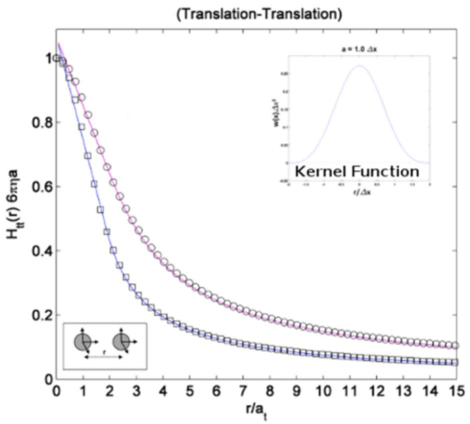
$$\langle \Gamma \mathbf{v}, \mathbf{F} \rangle = \sum_i [\Gamma \mathbf{v}]_i \cdot [\mathbf{F}]_i = \int_\Omega \mathbf{v}(\mathbf{x}) \cdot (\Lambda \mathbf{F})(\mathbf{x}) d\mathbf{x} = \langle \mathbf{v}, \Lambda \mathbf{F} \rangle$$

IB-Kernel coupling:

$$\Gamma \mathbf{u} = \int_\Omega \eta\left(\mathbf{y} - \mathbf{X}(t)\right) \mathbf{u}(\mathbf{y}, t) d\mathbf{y}$$

$$\Lambda \mathbf{F} = \eta\left(\mathbf{x} - \mathbf{X}(t)\right) \mathbf{F}.$$





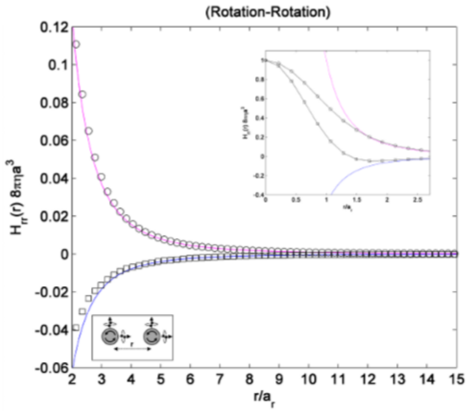
Generalized Coupling (Faxen)

$$\Gamma_0 \mathbf{u} = \sum_{\mathbf{m}} \left\langle\ \eta_0(\mathbf{y_m} - (\mathbf{X}_{cm} + \mathbf{z}))\ \mathbf{u_m}\ \right\rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \Delta x_{\mathbf{m}}^3$$

$$\Gamma_1 \mathbf{u} = \frac{3}{2R^2} \sum_{\mathbf{m}} \left\langle\ \eta_1(\mathbf{y_m} - (\mathbf{X}_{cm} + \mathbf{z}))\ (\mathbf{z} \times \mathbf{u_m})\ \right\rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \Delta x_{\mathbf{m}}^3.$$

$$\Lambda_0(\mathbf{x_m}) = \left(\left\langle\ \eta_0(\mathbf{x_m} - (\mathbf{X}_{cm} + \mathbf{z}))\ \right\rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \right) \mathbf{F}$$

$$\Lambda_1(\mathbf{x_m}) = -\frac{3}{2R^2} \left(\left\langle\ \mathbf{z}\eta_1(\mathbf{x_m} - (\mathbf{X}_{cm} + \mathbf{z}))\ \right\rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \right) \times \mathbf{T}.$$



Summary of Regimes for SELMs

Stochastic Eulerian Lagrangian Methods (SELMs)

Fluid dynamics:

$$\rho\frac{\partial \mathbf{u}}{\partial t} = \mu\Delta\mathbf{u} - \nabla p + \Lambda[\Upsilon(\mathbf{v} - \Gamma\mathbf{u})] + \mathbf{f}_{\mathrm{thm}}$$
$$\nabla\cdot\mathbf{u} = 0$$

Structure dynamics:

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Thermal Fluctuations

$$\langle \mathbf{f}_{\mathrm{thm}}(s)\mathbf{f}_{\mathrm{thm}}^T(t)\rangle = -(2k_BT)(\mu\Delta - \Lambda\Upsilon\Gamma)\,\delta(t-s)$$
$$\langle \mathbf{F}_{\mathrm{thm}}(s)\mathbf{F}_{\mathrm{thm}}^T(t)\rangle = (2k_BT)\,\Upsilon\,\delta(t-s)$$
$$\langle \mathbf{f}_{\mathrm{thm}}(s)\mathbf{F}_{\mathrm{thm}}^T(t)\rangle = -(2k_BT)\,\Lambda\Upsilon\,\delta(t-s).$$

Microstructure density matched with fluid

$m \ll \rho\ell^3$

Fluid-structure dynamics:

$$\frac{d\mathbf{p}}{dt} = \rho^{-1}\mathcal{L}\mathbf{p} + \Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\cdot\Lambda)\,k_BT + \lambda + \mathbf{g}_{\mathrm{thm}}$$
$$\frac{d\mathbf{X}}{dt} = \rho^{-1}\Gamma\mathbf{p} + \Upsilon^{-1}[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + \zeta + \mathbf{G}_{\mathrm{thm}}.$$
$$\nabla_{\mathbf{X}}\cdot\Lambda = \mathrm{Tr}[\nabla_{\mathbf{X}}\Lambda]$$

Phase space compressibility (p,X).

Thermal Fluctuations:

$$\langle \mathbf{g}_{\mathrm{thm}}(s)\mathbf{g}_{\mathrm{thm}}^T(t)\rangle = -(2k_BT)\,\mathcal{L}\,\delta(t-s)$$
$$\langle \mathbf{G}_{\mathrm{thm}}(s)\mathbf{G}_{\mathrm{thm}}^T(t)\rangle = (2k_BT)\,\Upsilon^{-1}\,\delta(t-s)$$
$$\langle \mathbf{g}_{\mathrm{thm}}(s)\mathbf{G}_{\mathrm{thm}}^T(t)\rangle = 0.$$

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

Microstructure-fluid no-slip coupling (S-Immersed-Boundary)

$\Upsilon \to \infty$

Fluid-Structure Equations:

$$\frac{d\mathbf{p}}{dt} = \rho^{-1}\mathcal{L}\mathbf{p} + \Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\cdot\Lambda)\,k_BT + \lambda + \mathbf{g}_{\mathrm{thm}}$$
$$\frac{d\mathbf{X}}{dt} = \rho^{-1}\Gamma\mathbf{p}$$

Thermal Fluctuations:

$$\langle \mathbf{g}_{\mathrm{thm}}(s)\mathbf{g}_{\mathrm{thm}}^T(t)\rangle = -(2k_BT)\,\mathcal{L}\,\delta(t-s).$$

- Structure dynamics no-longer inertial.
- Removes additional sources of stiffness.
- Regime of the Stochastic Immersed Boundary Method.
- Phase-space metric reflected in the drift term.

Microstructure-fluid stress balance

$\mu \to \infty$

Fluid-Structure Equations:

$$\frac{d\mathbf{X}}{dt} = H_{\mathrm{SELM}}[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\cdot H_{\mathrm{SELM}})k_BT + \mathbf{h}_{\mathrm{thm}}$$
$$H_{\mathrm{SELM}} = \Gamma(-\wp\mathcal{L})^{-1}\Lambda$$

Thermal Fluctuations:

$$\langle \mathbf{h}_{\mathrm{thm}}(s)\mathbf{h}_{\mathrm{thm}}^T(t)\rangle = (2k_BT)\,H_{\mathrm{SELM}}\,\delta(t-s).$$

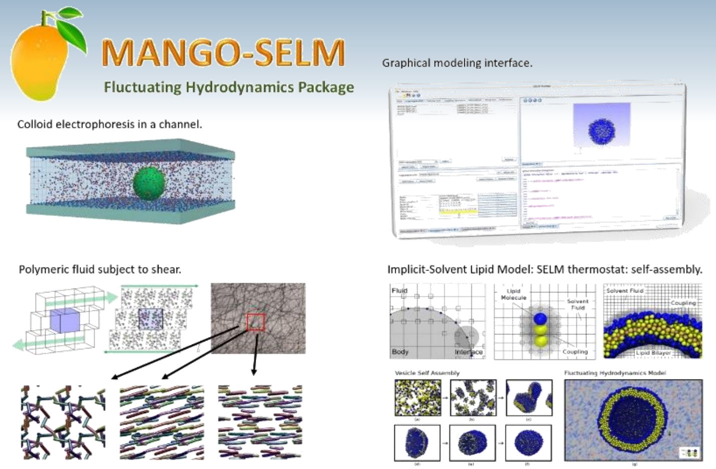
- Fluid momentum no longer tracked.
- Balance of hydrodynamic stresses with elastic stresses.
- Removes additional sources of stiffness.
- Regime of the Stokesian-Brownian Dynamics (Brady 1980, McCammond 1980's).
- Phase-space metric reflected in the drift term.

Atzberger & Tabak 2015

SELM-LAMMPS Integration

Molecular Dynamics and Coarse-Grained Modeling Approaches

Mango-Selm Software: Overview



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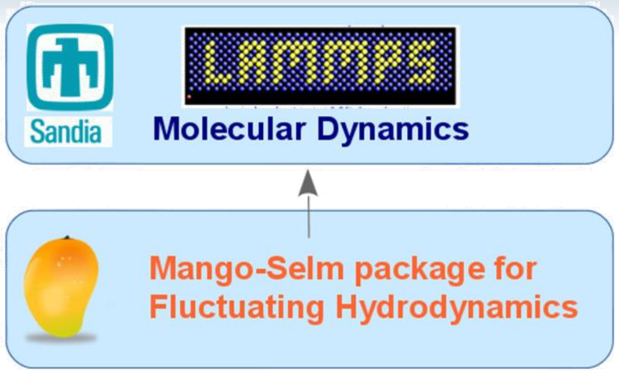

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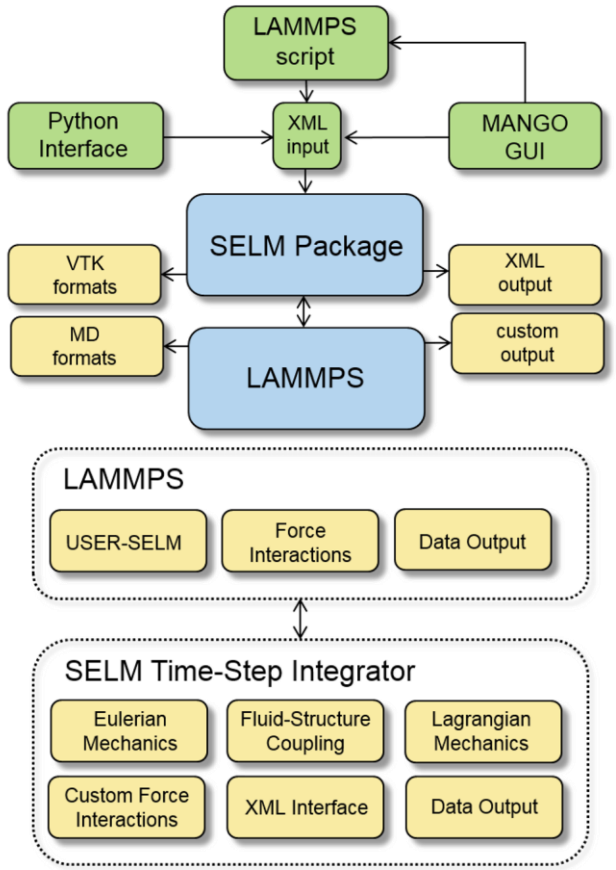

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Mango-Selm Implementation

Selm Codes: Design and Implementation

SELM – Source Codes:

LAMMPS-SELM Interface	XML Interface
fix_SELM.cpp	Atz_XML_Helper_ParseData.cpp
fix_SELM_XML_Handler.cpp	Atz_XML_Package.cpp
SELM_Package.cpp	Atz_XML_Parser.cpp
Atz_XML_Handler_Example_A.cpp	Atz_XML_SAX_DataHandler.cpp
Atz_XML_Helper_DataHandler_List.cpp	Atz_XML_SAX_Handler_Multilevel.cpp
Atz_XML_Helper_Handler_SkipNextTag.cpp	Atz_XML_SAX_Handler_PrintToScreen.cpp
Eulerian Mechanics	**Lagrangian Mechanics**
SELM_Eulerian.h	SELM_Lagrangian.h
SELM_Eulerian_Types.h	SELM_Lagrangian_Delegator_XML_Handler.h
SELM_Eulerian_Delegator_XML_Handler.h	SELM_Lagrangian_LAMMPS_ATOM_ANGLE_STYLE.h
SELM_Eulerian_LAMMPS_SHEAR_UNIFORM1_FFTW3.h	SELM_Lagrangian_LAMMPS_ATOM_ANGLE_STYLE_XML_Handler.h
SELM_Eulerian_LAMMPS_SHEAR_UNIFORM1_FFTW3_XML_Handler.h	SELM_Lagrangian_Types.h
SELM_Eulerian_Uniform1_Periodic.h	SELM_Package.h
SELM_Eulerian_Uniform1_Periodic_XML_Handler.h	
Time-Step Integration	**Fluid-Structure Coupling**
SELM_Integrator.h	SELM_CouplingOperator.h
SELM_Integrator_Delegator_XML_Handler.h	SELM_CouplingOperator_Delegator_XML_Handler.h
SELM_Integrator_FFTW3_Period.h	SELM_CouplingOperator_LAMMPS_SHEAR_UNIFORM1_FFTW3_TABLE1.h
SELM_Integrator_LAMMPS_SHEAR_QUASI_STEADY1_FFTW3.h	SELM_CouplingOperator_LAMMPS_SHEAR_UNIFORM1_FFTW3_TABLE1_XML_Handler.h
SELM_Integrator_LAMMPS_SHEAR_QUASI_STEADY1_FFTW3_XML_Handler.h	

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.

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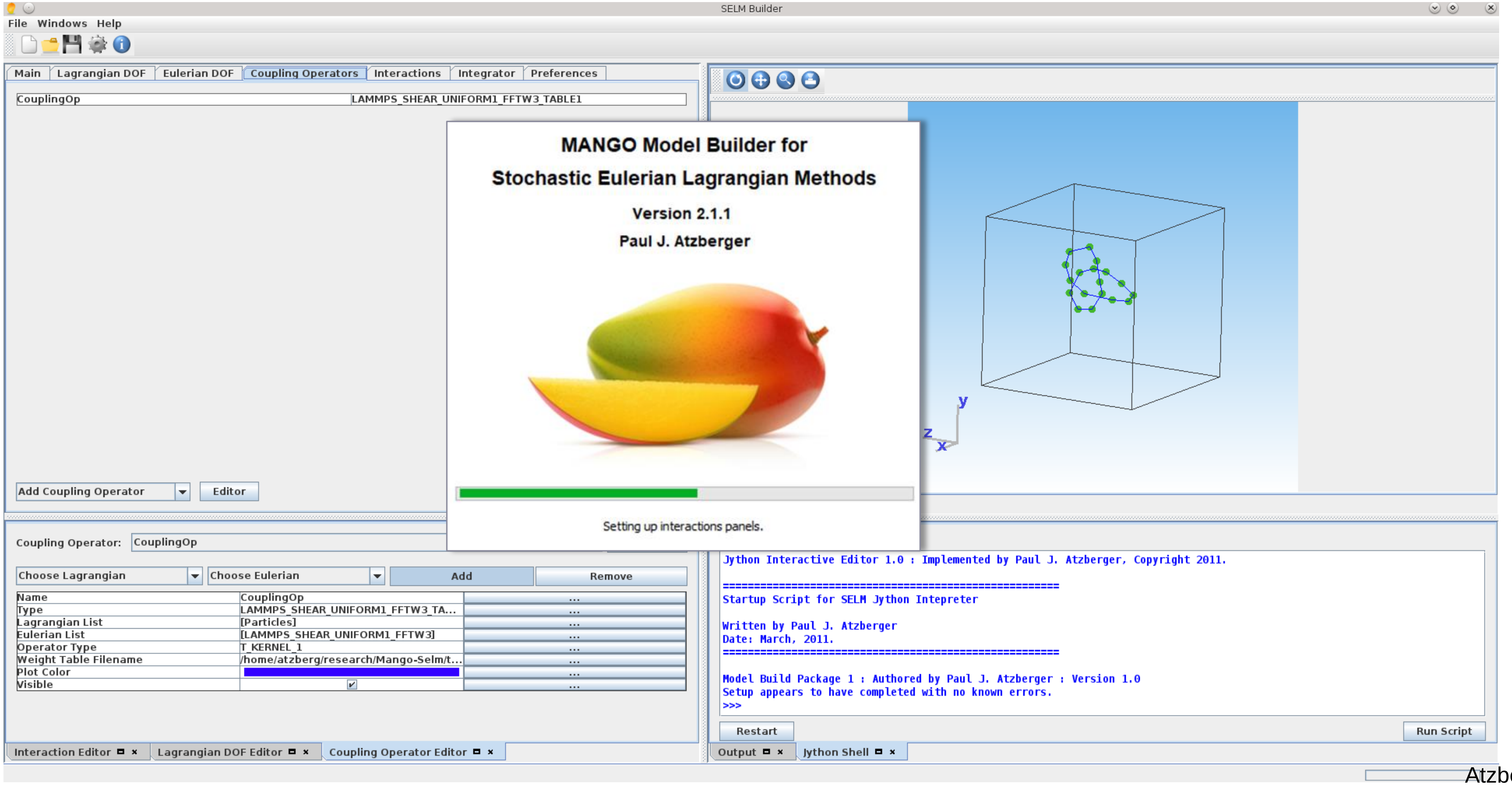
Mango GUI Model Builder

Mango - Modeling Software:



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Mango Modeling Software

Mango - Codes

SELM-Builder		
application_Main.java	JPanel_Lagrangian.java	SELM_RenderView.java
application_Project_Atz_XML_DataHandler_LAMMPS_USER_SELM.java	JPanel_Lagrangian_CONTROL_PTS_BASIC1.java	TableData_CouplingOperatorList.java
application_Project_Atz_XML_DataHandler_SELM_Builder.java	JPanel_Lagrangian_CONTROL_PTS_FAXEN1.java	TableData_EulerianList.java
application_SharedData.java	JPanel_Lagrangian_LAMMPS_ATOM_ANGLE_STYLE.java	TableData_EulerianList_old.java
application_Window_About.java	JPanel_Lagrangian_NULL.java	TableData_IntegratorList.java
application_Window_Main.java	JPanel_Lagrangian_SPECTRAL_FILAMENT1.java	TableData_InteractionList.java
application_Window_Main_SetupThread.java	JTable_CouplingOperator_LAMMPS_SHEAR_UNIFORM1_FFTW3_TABLE1.java	TableData_LagrangianList.java
application_Window_Splash.java	JTable_Interaction.java	TableData_LAMMPS_pair_coeff_tableFilename.java
Atz_Application_Data_Communication.java	JTable_Interaction_LAMMPS_ANGLES.java	TableEditor_CouplingOperatorList.java
Atz_ClassLoader.java	JTable_Interaction_LAMMPS_BONDS.java	TableEditor_EulerianList.java
Atz_ClassLoader_RegistryInfo.java	JTable_Interaction_LAMMPS_CUSTOM1.java	TableEditor_IntegratorList.java
Atz_DataChangeable.java	JTable_Interaction_LAMMPS_PAIR_COEFF.java	TableEditor_InteractionList.java
Atz_DataChangeEvent.java	JTable_Interaction_LAMMPS_PAIRS_HARMONIC.java	TableEditor_LagrangianList.java
Atz_DataChangeListener.java	JTable_Interaction_LAMMPS_SPECIAL_BONDS.java	TableEditor_LAMMPS_PAIR_COEFF_tableFilename.java
Atz_File_Generator.java	JTable_Interaction_PAIRS_HARMONIC.java	TableModel_CouplingOperator.java
Atz_File_Generator_LAMMPS_USER_SELM1.java	JTable_Lagrangian_ControlPts_BASIC1.java	TableModel_CouplingOperator_IB1.java
Atz_FileFilter.java	JTable_Langrangian_CONTROL_PTS.java	TableModel_CouplingOperator_LAMMPS_SHEAR_UNIFORM1_FFTW3_TABLE1.java
Atz_Helper_Generic.java	JTable_MainData.java	TableModel_CouplingOperator_TABLE1_tmp.java
Atz_Object_Factory.java	JTable_MainData_XML_LAMMPS_USER_SELM.java	TableModel_CouplingOperatorList.java
Atz_Object_Factory_Generic.java	JTable_MainData_XML_SELM_Builder.java	TableModel_Eulerian.java
Atz_Struct_DataChangeEvent.java	JTable_Preferences_Other.java	TableModel_Eulerian_LAMMPS_SHEAR_UNIFORM1_FFTW3.java
Atz_Struct_DataChangeListener.java	JTable_Preferences_Rendering.java	TableModel_Eulerian_SHEAR_UNIFORM1_FFTW3.java
Atz_Struct_DataChangeListener_MainData.java	JTable_Preferences_TableDisplay.java	TableModel_Eulerian_SHEAR_UNIFORM1_FFTW3_old.java
Atz_Struct_DataChangeListener_Test1.java	JTableHeaderRender_Default1.java	TableModel_Integrator.java
Atz_Struct_DataContainer.java	SELM_CouplingOperator.java	TableModel_Integrator_LAMMPS_SHEAR_QUASI_STEADY1_FFTW3.java
Atz_Struct_DataContainer_MainData.java	SELM_CouplingOperator_IB1.java	TableModel_Integrator_LAMMPS_SHEAR1.java
Atz_Struct_DataListManager.java	SELM_CouplingOperator_LAMMPS_SHEAR_UNIFORM1_FFTW3_TABLE1.java	TableModel_Integrator_SELM_SHEAR1_old.java
Atz_XML_Helper_Handler_EulerianRef.java	SELM_CouplingOperator_NULL.java	TableModel_Integrator_SHEAR1.java
Atz_XML_Helper_Handler_LagrangianRef.java	SELM_CouplingOperator_XML_DataDelegator.java	TableModel_Interaction.java
JDialog_Edit_CouplingOperatorList.java	SELM_Eulerian.java	TableModel_Interaction_LAMMPS_ANGLES.java
JDialog_Edit_EulerianList.java	SELM_Eulerian_LAMMPS_SHEAR_UNIFORM1_FFTW3.java	TableModel_Interaction_LAMMPS_BONDS.java
JDialog_Edit_InteractionList.java	SELM_Eulerian_NULL.java	TableModel_Interaction_LAMMPS_CUSTOM1.java
JDialog_Edit_LagrangianList.java	SELM_Eulerian_SHEAR_UNIFORM1_FFTW3.java	TableModel_Interaction_LAMMPS_PAIR_COEFF.java
JDialog_FontSelector.java	SELM_Eulerian_UNIFORM1_FFTW3.java	TableModel_Interaction_LAMMPS_PAIRS_HARMONIC.java
JDialog_Generate_Simulation_Data_LAMMPS.java	SELM_Eulerian_XML_DataDelegator.java	TableModel_Interaction_LAMMPS_SPECIAL_BONDS.java
JDialog_Message_Generate_LAMMPS_USER_SELM.java	SELM_EulerianInterface_LAMMPS.java	TableModel_InteractionList.java
JFrame_SplashProgress.java	SELM_EulerianRenderView.java	TableModel_Lagrangian.java
JPanel_CouplingOperator.java	SELM_Integrator.java	TableModel_Lagrangian_CONTROL_PTS_BASIC1.java
JPanel_CouplingOperator_IB1.java	SELM_Integrator_BD1.java	TableModel_Lagrangian_CONTROL_PTS_FAXEN1.java
JPanel_CouplingOperator_LAMMPS_SHEAR_UNIFORM1_FFTW3_TABLE1.java	SELM_Integrator_LAMMPS_SHEAR_QUASI_STEADY1_FFTW3.java	TableModel_Lagrangian_LAMMPS_ATOM_ANGLE_STYLE.java
JPanel_CouplingOperator_NULL.java	SELM_Integrator_LAMMPS_SHEAR1.java	TableModel_Lagrangian_SPECTRAL_FILAMENT1.java
JPanel_Demo1.java	SELM_Integrator_NULL.java	TableModel_LagrangianList.java
JPanel_Edit_CouplingOpList.java	SELM_Integrator_SHEAR1.java	TableModel_MainData.java
JPanel_Edit_InteractionList.java	SELM_Integrator_XML_DataDelegator.java	TableModel_Preferences_Other.java
JPanel_Edit_LagrangianList.java	SELM_IntegratorInterface_LAMMPS.java	TableModel_Preferences_Rendering.java
JPanel_Editor_CouplingOperator.java	SELM_IntegratorRenderView.java	TableModel_Preferences_TableDisplay.java
JPanel_Editor_Eulerian_DOF.java	SELM_Interaction.java	TableModel_Properties1_Test1.java
JPanel_Editor_Integrator.java	SELM_Interaction_LAMMPS_ANGLES.java	TableRenderer_CouplingOperatorList.java
JPanel_Editor_Interaction.java	SELM_Interaction_LAMMPS_BONDS.java	TableRenderer_EulerianList.java
JPanel_Editor_Lagrangian_DOF.java	SELM_Interaction_LAMMPS_CUSTOM1.java	TableRenderer_IntegratorList.java
JPanel_Editor_Test1.java	SELM_Interaction_LAMMPS_PAIR_COEFF.java	TableRenderer_InteractionList.java
JPanel_Eulerian.java	SELM_Interaction_LAMMPS_PAIRS_HARMONIC.java	TableRenderer_LagrangianList.java
JPanel_Eulerian_interface_controlActionListener.java	SELM_Interaction_LAMMPS_SPECIAL_BONDS.java	TableRenderer_LAMMPS_pair_coeff_tableFilename.java
JPanel_Eulerian_LAMMPS_SHEAR_UNIFORM1_FFTW3.java	SELM_Interaction_NULL.java	XMLContentHandler.java
JPanel_Eulerian_NULL.java	SELM_Interaction_PAIRS_HARMONIC.java	3D Rendering
JPanel_Eulerian_SHEAR_UNIFORM1_FFTW3.java	SELM_Interaction_PAIRS_TABLE.java	Atz_LinearAlgebra.java
JPanel_Eulerian_UNIFORM1_FFTW3.java	SELM_Interaction_TARGET1.java	Atz3D_Camera.java
JPanel_Helper_CouplingOperator_GenericTable.java	SELM_Interaction_XML_DataDelegator.java	Atz3D_Element.java
JPanel_Helper_Eulerian_GenericTable.java	SELM_InteractionInterface_LAMMPS.java	Atz3D_Element_LinePairs.java
JPanel_Helper_Integrator_GenericTable.java	SELM_InteractionInterface_LAMMPS_ANGLES.java	Atz3D_Element_Lines.java
JPanel_Helper_Interaction_GenericTable.java	SELM_InteractionInterface_LAMMPS_BONDS.java	Atz3D_Element_Points.java
JPanel_Helper_Lagrangian_GenericTable.java	SELM_InteractionInterface_LAMMPS_PAIR_STYLE.java	Atz3D_Element_Points_DataClosest.java
JPanel_Integrator.java	SELM_InteractionInterface_LAMMPS_PAIR_STYLE_TABLE.java	Atz3D_Model.java
JPanel_Integrator_BD1.java	SELM_InteractionRenderView.java	Atz3D_Model_SELM.java
JPanel_Integrator_LAMMPS_SHEAR_QUASI_STEADY1_FFTW3.java	SELM_Lagrangian.java	Atz3D_Renderer.java
JPanel_Integrator_NULL.java	SELM_Lagrangian_CONTROL_PTS_BASIC1.java	Atz3D_Renderer_SELM.java
JPanel_Interaction.java	SELM_Lagrangian_CONTROL_PTS_FAXEN1.java	JPanel_Model_View_Composite.java
JPanel_Interaction_LAMMPS_ANGLES.java	SELM_Lagrangian_interface.java	JPanel_Model_View_Composite_XML_SELM_Builder.java
JPanel_Interaction_LAMMPS_BONDS.java	SELM_Lagrangian_LAMMPS_ATOM_ANGLE_STYLE.java	JPanel_Model_View_RenderPanel.java
JPanel_Interaction_LAMMPS_CUSTOM1.java	SELM_Lagrangian_NULL.java	JPanel_Model_View_RenderPanel_XML_SELM_Builder.java
JPanel_Interaction_LAMMPS_PAIR_COEFF.java	SELM_Lagrangian_SPECTRAL_FILAMENT1.java	Physical Units
JPanel_Interaction_LAMMPS_PAIRS_HARMONIC.java	SELM_Lagrangian_wrapper.java	Atz_Unit.java
JPanel_Interaction_LAMMPS_SPECIAL_BONDS.java	SELM_Lagrangian_XML_DataDelegator.java	Atz_UnitsData.java
JPanel_Interaction_NULL.java	SELM_LagrangianInterface_LAMMPS.java	Atz_UnitsRef.java
JPanel_Interaction_PAIRS_HARMONIC.java	SELM_LagrangianRef_XML_DataHandler.java	Atz_UnitsRef_PhysicalUnits.java
JPanel_Interaction_TARGET1.java	SELM_LagrangianRenderView.java	JDialog_Edit_Units_Ref.java

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Mango Modeling Software

MANGO - Codes

SELM-Builder	
application_Main.java	JPanel_Lagrangian.java
application_Project_Atz_XML_DataHandler_LAMMPS_USER_SELM.java	JPanel_Lagrangian_CONTROL_PTS_BASIC1.java
application_Project_Atz_XML_DataHandler_SELM_Builder.java	JPanel_Lagrangian_CONTROL_PTS_FAXEN1.java
application_SharedData.java	JPanel_Lagrangian_LAMMPS_ATOM_ANGLE_STYLE.java
application_Window_About.java	JPanel_Lagrangian_NULL.java
application_Window_Main.java	JPanel_Lagrangian_SPECTRAL_FILAMENT1.java
application_Window_Main_SetupThread.java	JTable_CouplingOperator_LAMMPS_SHEAR_UNIFORM1_FFTW3_TABLE1.java
application_Window_Splash.java	JTable_Interaction.java
Atz_Application_Data_Communication.java	JTable_Interaction_LAMMPS_ANGLES.java
Atz_ClassLoader.java	JTable_Interaction_LAMMPS_BONDS.java
Atz_ClassLoader_RegistryInfo.java	JTable_Interaction_LAMMPS_CUSTOM1.java
Atz_DataChangeable.java	JTable_Interaction_LAMMPS_PAIR_COEFF.java
Atz_DataChangeEvent.java	JTable_Interaction_LAMMPS_PAIRS_HARMONIC.java
Atz_DataChangeListener.java	JTable_Interaction_LAMMPS_SPECIAL_BONDS.java
Atz_File_Generator.java	JTable_Interaction_PAIRS_HARMONIC.java
Atz_File_Generator_LAMMPS_USER_SELM1.java	JTable_Lagrangian_ControlPts_BASIC1.java
Atz_FileFilter.java	JTable_Langrangian_CONTROL_PTS.java
Atz_Helper_Generic.java	JTable_MainData.java
Atz_Object_Factory.java	JTable_MainData_XML_LAMMPS_USER_SELM.java
Atz_Object_Factory_Generic.java	JTable_MainData_XML_SELM_Builder.java
Atz_Struct_DataChangeEvent.java	JTable_Preferences_Other.java
Atz_Struct_DataChangeListener.java	JTable_Preferences_Rendering.java
Atz_Struct_DataChangeListener_MainData.java	JTable_Preferences_TableDisplay.java

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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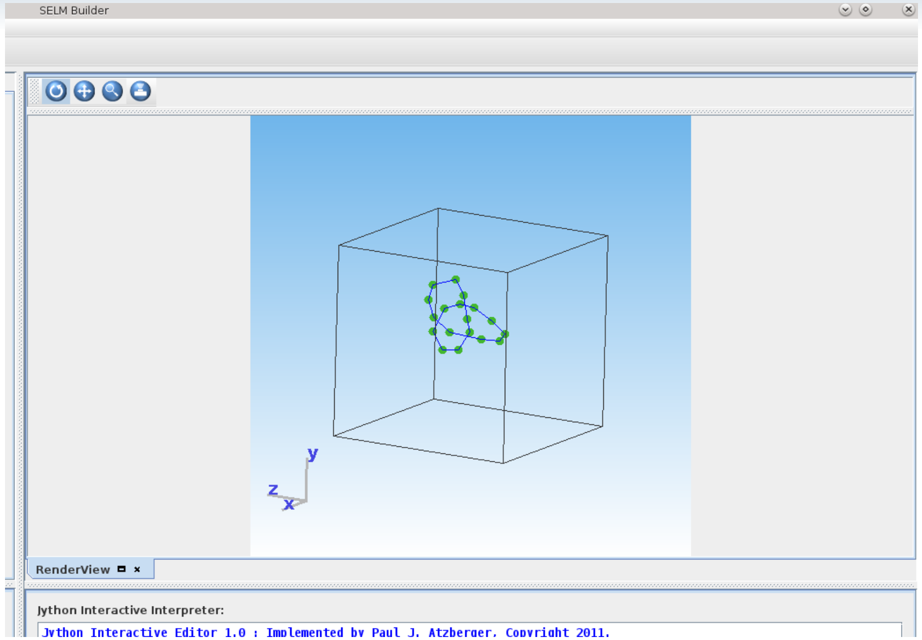
Mango Modeling Software

Mango – Codes:

3D Rendering
Atz_LinearAlgebra.java
Atz3D_Camera.java
Atz3D_Element.java
Atz3D_Element_LinePairs.java
Atz3D_Element_Lines.java
Atz3D_Element_Points.java
Atz3D_Element_Points_DataClosest.java
Atz3D_Model.java
Atz3D_Model_SELM.java
Atz3D_Renderer.java
Atz3D_Renderer_SELM.java
JPanel_Model_View_Composite.java
JPanel_Model_View_Composite_XML_SELM_Builder.java
JPanel_Model_View_RenderPanel.java
JPanel_Model_View_RenderPanel_XML_SELM_Builder.java
Physical Units
Atz_Unit.java
Atz_UnitsData.java
Atz_UnitsRef.java
Atz_UnitsRef_PhysicalUnits.java
JDialog_Edit_Units_Ref.java



Features:

Rendering in 3D for interactively editing for model geometry.
Interactive editor features allow for

- interactive views of model
- adding / removing control points
- adding / removing bonds between points
- adding custom force interactions

Custom classes implemented for tracking physical units in tables.

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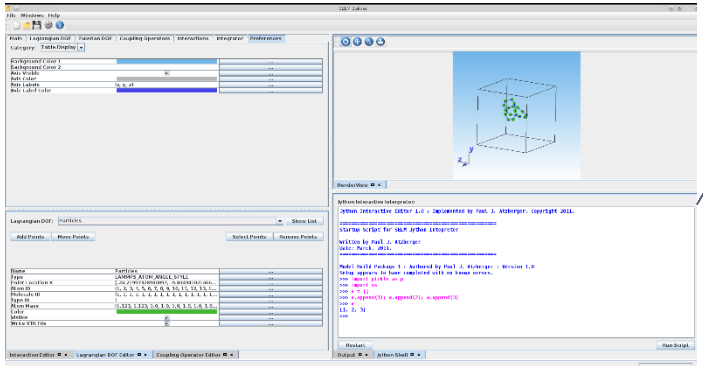
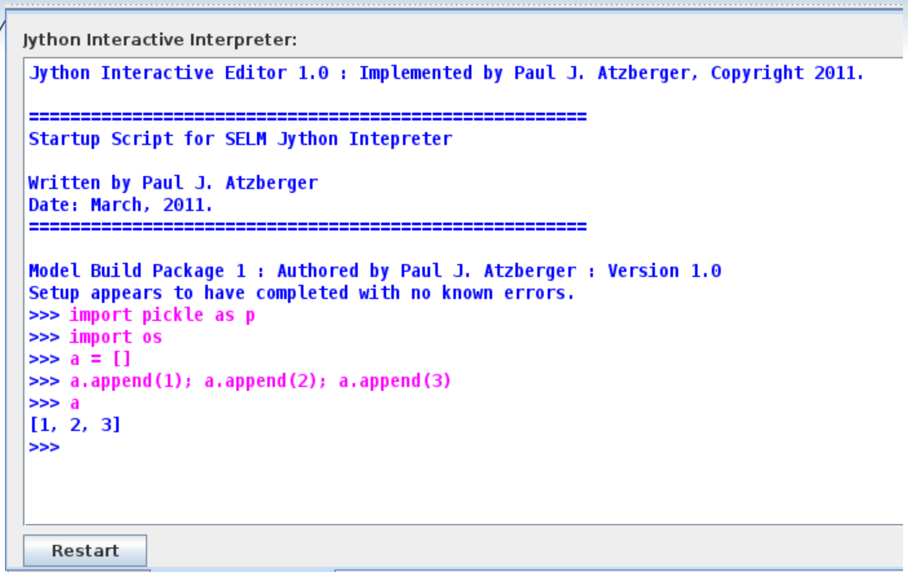
Mango GUI Jython Interface

MANGO - Modeling Software:





Jython Terminal:

Custom classes implement interactive terminal based on Jython.
Wrapper jython classes implemented for MANGO interface and SELM data structures.
Editor features allow for

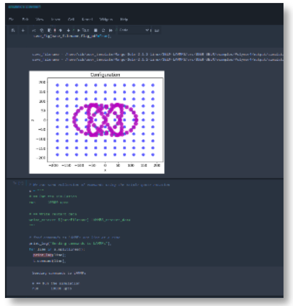
- jython/python scripting to construct models
- custom GUI windows : interactive components in MANGO
- post-processing scripts
- generation of SELM XML files from the constructed MANGO data structures.

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

Python and Jupyter notebook interfaces

jupyter

python



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Selm-Lammps Integration

Python and Jupyter Notebook Interfaces

Tips for SELM Package: Installation and Usage

Instructions

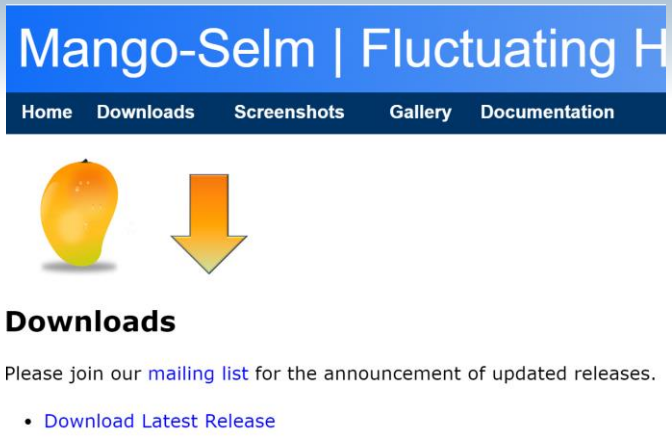
Download at: http://mango-selm.org/

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

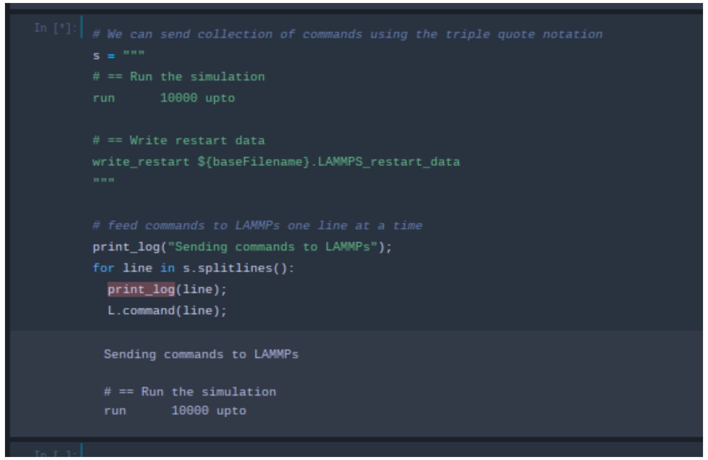
Installing Python components (uses lammps.py, lammps.so):
- Conda or virtualenv determine dir by “which python”
- Copy shared library and files into XX/site-packages/ directory.
- Create symbolic links to the shared library and binaries (or put in path)
  - ln –s XXX/bin/lammps.so lammps.so
- See examples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



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

Python and Jupyter notebook interfaces



Jupyter Notebook and Python Interface

Python Jupyter Notebook

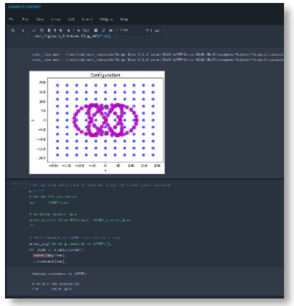
```
simulation_polymer4
File  Edit  View  Insert  Cell  Kernel  Widgets  Help
Run  Markdown
```

SELM via PyLAMMPs for Simulations

Author: Paul Atzberger

http://atzberger.org/

Python and Jupyter notebook interfaces



Create Selm-Lammps instance

Setup LAMMPs

```
In [10]:  L = IPyLammps()
          print_version_info();

LAMMPS output is captured by PyLammps wrapper
LAMMPS version: 29 Oct 2020 / 20201029
MPI version: LAMMPS MPI STUBS for LAMMPS version 29 Oct 2020
```

Issuing commands

```
In [ ]:   cmd_str = "lammps_command"
          L.command(cmd_str);
```

Setup model geometry and interactions

Setup the Simulation Files (such as .read_data)

```
In [13]:  num_dim = 3;
          box = np.zeros((num_dim,2));
          LL = 202.5; box[:,0] = -LL; box[:,1] = LL;

          # setup atoms
          I_id = 1; I_type = 1; atom_types = [];
          atom_list = []; atom_mass_list = []; atom_id_list = [];
          atom_mol_list = []; atom_name_list = [];

          # polymer atoms
          atom_name = "polymer_pts";
          atom_name_list.append(atom_name);
          atom_types.append(I_type);
```

```
num_pts = 100;
t = np.linspace(0,2*np.pi,num_pts); R0 = 40;
x1 = R0*(2.0 + np.cos(2.0*t))*np.cos(3.0*t);
x2 = R0*(2.0 + np.cos(2.0*t))*np.sin(3.0*t);
x3 = R0*2*np.sin(4.0*t);
x = np.stack((x1,x2,x3),axis=1); # shape = [num_pts,num_dim]
num_pts = x.shape[0]; m0 = 1.123;
```

→

Model configuration (generated file)

```
# ===========================================================================
# LAMMPS file for 'read_data' command
#
# Generated by selm python scripts by Paul J. Atzberger.
#
# ===========================================================================

# ===========================================================================
# Description:
# ---------------------------------------------------------------------------
#
# SELM_Lagrangian = SELM_Lagrangian_LAMMPS_ATOM_ANGLE_STYLE
# LagrangianName = Points
# LagrangianTypeStr = LAMMPS_ATOM_ANGLE_STYLE
#
# SELM_Eulerian   = SELM_Eulerian_LAMMPS_SHEAR_UNIFORM1_FFTW3
#
# atom_type = angle_type
#
# ===========================================================================

# ===========================================================================
# Header information:
# ---------------------------------------------------------------------------
1431 atoms
99 bonds
98 angles

2 atom types
1 bond types
1 angle types
# ===========================================================================

# ===========================================================================
# Domain Size Specification:
# ---------------------------------------------------------------------------
-202 202 xlo xhi
-202 202 ylo yhi
```

→

Setup parameters

```
# We can send collection of commands using the triple quote notation
s = """
# ===========================================================================
# LAMMPS main parameter file and script
#
# Author: Paul J. Atzberger.
#
# Based on script generated by MANGO-SELM Model Builder.
#
# ===========================================================================

# == Setup variables for the script

variable dumpfreq         equal    1
variable restart          equal    0
variable neighborSkinDist equal    1.0 # distance for bins beyond force cut-off (1.0 = 1.0
variable baseFilename     universe Polymer

# == Setup the log file
#log         ${baseFilename}.LAMMPS_logFile

# == Setup style of the run

# type of units to use in the simulation (units used are in fact: amu, nm, ns, Kelvins)
units       real

# indicates possible types allowed for interactions between the atoms
atom_style  angle

# indicates possible types allowed for bonds between the atoms
#bond_style  hybrid fene
bond_style hybrid harmonic
```

SELM XML files

→

Run simulation and analysis

```
In [20]:  # We can send collection of commands using the triple quote notation
          s = """
          # == Run the simulation
          run      1000 upto

          # == Write restart data
          write_restart ${baseFilename}.LAMMPS_restart_data
          """

          # feed commands to LAMMPS one line at a time
          print_log("Sending commands to LAMMPs");
          for line in s.splitlines():
            print_log(line);
            L.command(line);
```

Interface allows for:

- checking intermediate results
- resuming simulations
- perform 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 LAMMPs

```
In [10]:
L = IPyLammps()
print_version_info();
```

```
LAMMPS output is captured by PyLammps wrapper
LAMMPS version: 29 Oct 2020 / 20201029
MPI version: LAMMPS MPI STUBS for LAMMPS version 29 Oct 2020
```

Setup model geometry and interactions

Setup the Simulation Files (such as .read_data)

```
In [13]:
num_dim = 3;
box = np.zeros((num_dim,2));
LL = 202.5; box[:,0] = -LL; box[:,1] = LL;

# setup atoms
I_id = 1; I_type = 1; atom_types = [];
atom_list = []; atom_mass_list = []; atom_id_list = [];
atom_mol_list = []; atom_name_list = [];

# polymer atoms
atom_name = "polymer_pts";
atom_name_list.append(atom_name);
atom_types.append(I_type);
```

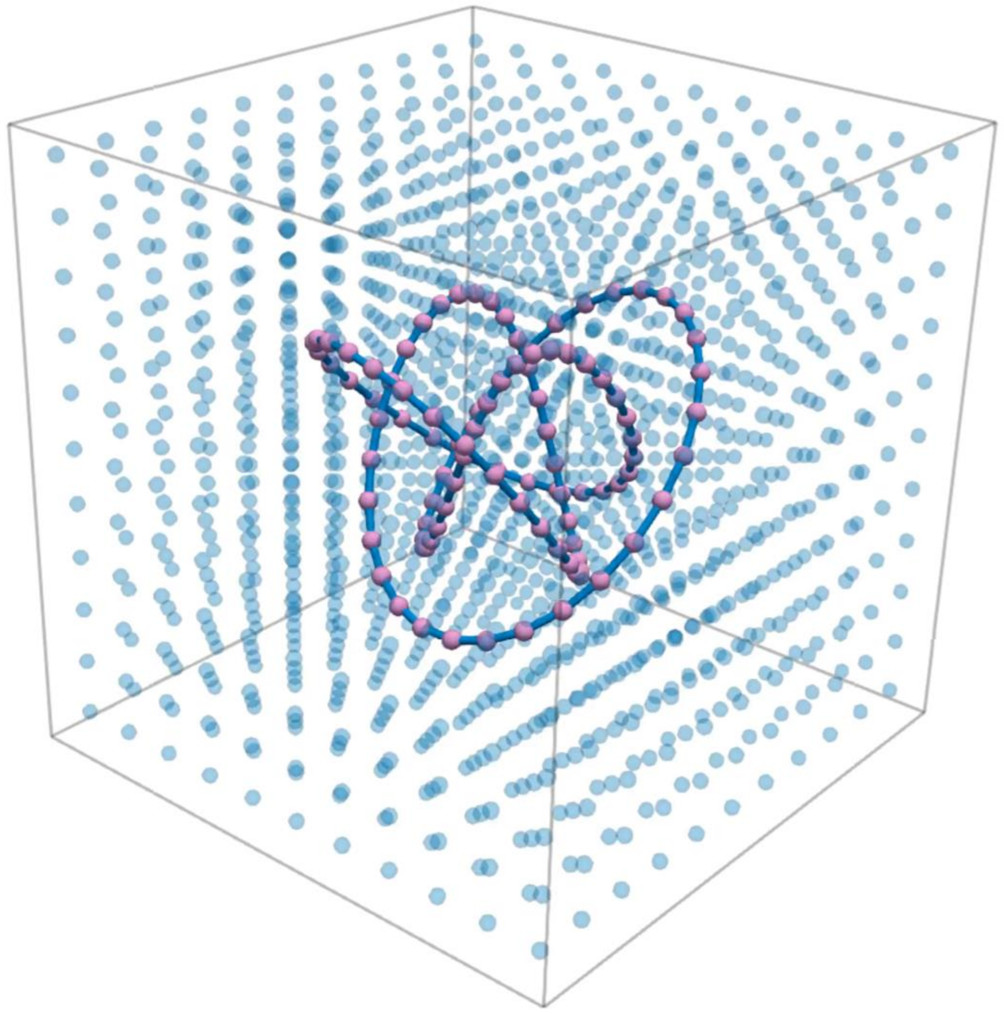
```
num_pts = 100;
t = np.linspace(0,2*np.pi,num_pts); R0 = 40;
x1 = R0*(2.0 + np.cos(2.0*t))*np.cos(3.0*t);
x2 = R0*(2.0 + np.cos(2.0*t))*np.sin(3.0*t);
x3 = R0*2*np.sin(4.0*t);
x = np.stack((x1,x2,x3),axis=1); # shape = [num_pts,num_dim]
num_pts = x.shape[0]; m0 = 1.123;
```

→

Run simulation and analysis

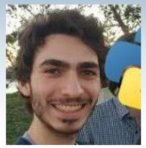
```
In [20]:
# We can send collection of commands using the triple quote notation
s = """
# == Run the simulation
run      1000 upto

# == Write restart data
write_restart ${baseFilename}.LAMMPS_restart_data
"""

# feed commands to LAMMPs one line at a time
print_log("Sending commands to LAMMPs");
for line in s.splitlines():
  print_log(line);
  L.command(line);
```

SELM XML files



Conclusions

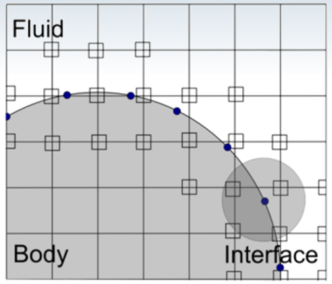

B. Gross

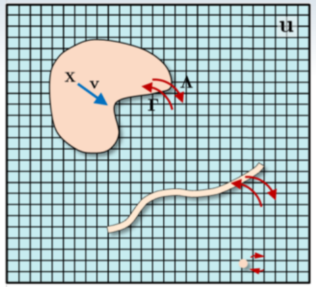

D. Rower

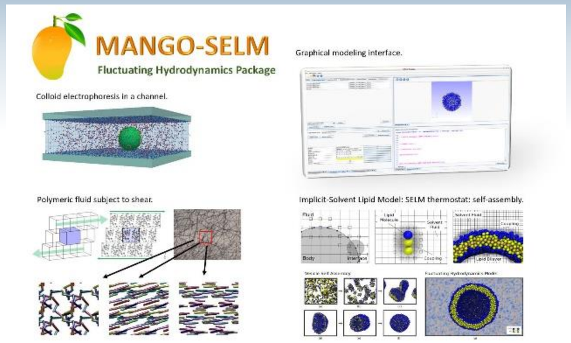

M. Padidar


J. Sigurdsson

UCSB Recent Student Collaborators







Paper
2016 Atzberger & Sigurdsson

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.*

Mango-Selm package for Fluctuating Hydrodynamics
http://atzberger.org

Papers

A Stochastic Immersed Boundary Method for Fluid-Structure Dynamics at Microscopic Length Scales,
P.J. Atzberger, P.R. Kramer, and C.S. Peskin, J. Comp. Phys., Vol. 224, Iss. 2, (2007).

Stochastic Eulerian Lagrangian Methods for Fluid Structure Interactions with Thermal Fluctuations,
P.J. Atzberger, J. of Comp. Phys., 230, pp. 2821--2837, (2011).

Surface Fluctuating Hydrodynamics Methods for the Drift-Diffusion Dynamics of Particles and Microstructures within Curved Fluid Interfaces,
D. Rower, M. Padidar, and P. J. Atzberger, arXiv:1906.01146, (2019).

Meshfree Methods on Manifolds for Hydrodynamic Flows on Curved Surfaces: A Generalized Moving Least-Squares (GMLS) Approach,
Gross B. J., Kuberry P. A., Trask N., Atzberger P. J., J. Comp. Phys., 409, 15 May (2020).

UCSB Recent Student Collaborators

B. Gross, M. Padidar, D. Rower, J. K. Sigurdsson.

Sandia Collaborators

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

Funding

DOE ASCR CM4
DE-SC0009254

DOE ASCR PhILMS
DE-SC0019246

NSF Grant
DMS - 1616353

NSF CAREER Grant
DMS-0956210

More information: http://atzberger.org/

Publications

A Stochastic Immersed Boundary Method for Fluid-Structure Dynamics at Microscopic Length Scales,
P.J. Atzberger, P.R. Kramer, and C.S. Peskin, J. Comp. Phys., Vol. 224, Iss. 2, (2007). http://dx.doi.org/10.1016/j.jcp.2006.11.015

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