Fluctuating Hydrodynamics Approaches for Mesoscopic Modeling and Simulation
Applications in Soft Materials and Fluidics

Computational Methods and Software

Summer School on Multiscale Modeling of Materials
Stanford University
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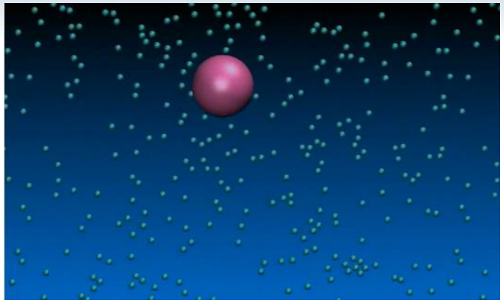
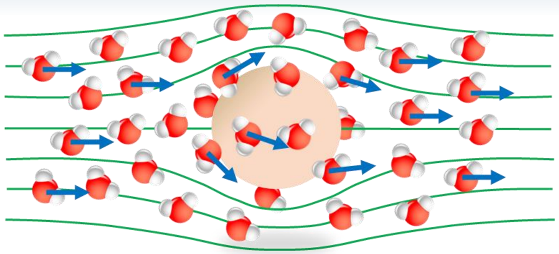
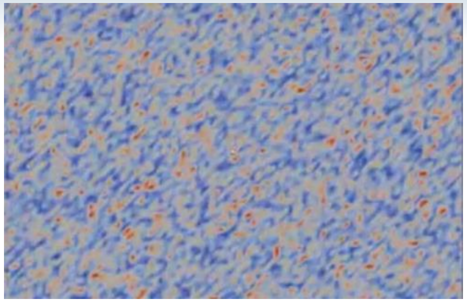
Fluctuating Hydrodynamics



Brownian Motion: Molecular Collisions



Hydrodynamics + Fluctuations



Continuum Gaussian Random Field

Landau-Lifschitz fluctuating hydrodynamics

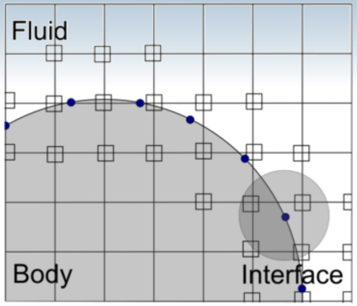
$$\rho\left(\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + \mathbf{u}(\mathbf{x},t)\cdot\nabla\mathbf{u}(\mathbf{x},t)\right) = \mu\Delta\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \nabla\cdot\mathbf{\Sigma}(\mathbf{x},t).$$

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

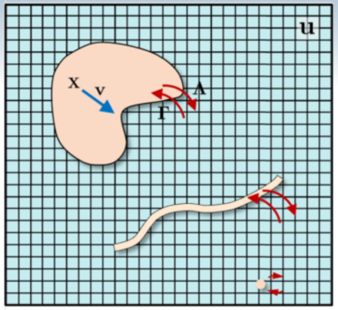
$$\langle\Sigma_{ij}(\mathbf{x},t)\Sigma_{kl}(\mathbf{y},s)\rangle = 2\mu k_B T\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\delta(\mathbf{x}-\mathbf{y})\delta(t-s).$$

- Spontaneous momentum transfer from molecular-level interactions.
- Thermal fluctuations captured through random stress Σ.
- Mathematically, equations present challenges since δ-correlation in space-time.
- Fluid-structure interactions?

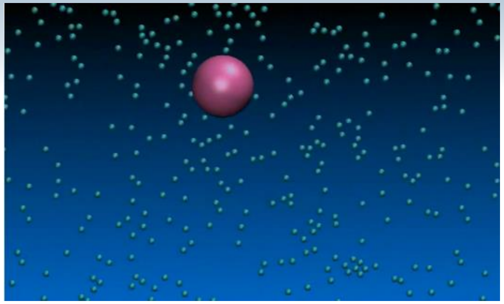
SELM Fluctuating Hydrodynamics



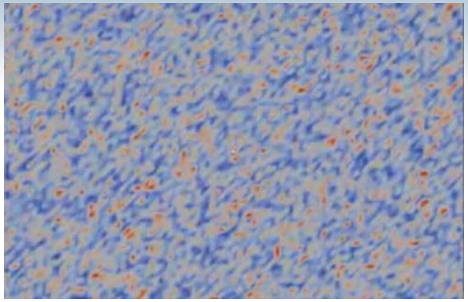
Eulerian-Lagrangian Mechanics



Eulerian-Lagrangian Coupling



Brownian Motion: Molecular Collisions



Continuum Gaussian Random Field

SELM Inertial Regime I:

hydrodynamics

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

microstructure

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

thermal fluctuations

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

SELM Overdamped Regime IV:

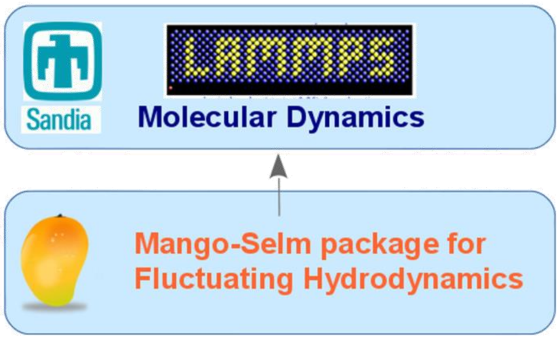
microstructure + hydrodynamics (quasi-steady)

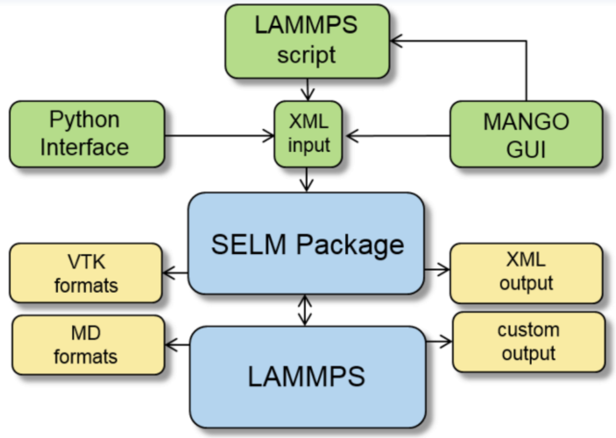
$$\begin{aligned} \frac{d\mathbf{X}}{dt} &= H_{\mathrm{SELM}}[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] \\ &+ (\nabla_{\mathbf{X}}\cdot H_{\mathrm{SELM}})k_BT + \mathbf{h}_{\mathrm{thm}} \\ H_{\mathrm{SELM}} &= \Gamma(-\wp\mathcal{L})^{-1}\Lambda \end{aligned}$$

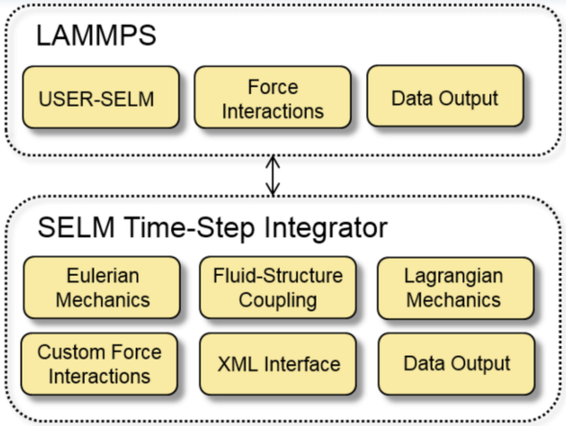
thermal fluctuations

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

MANGO-SELM Simulation Software







MANGO-SELM Software Features:

SELM - Simulation Software:

- SELM fluctuating hydrodynamics : fluid-structure interactions subject to thermal fluctuations.
- Numerical time-step integrators for inertial and quasi-steady physical regimes(C/C++).
- Lees-Edwards-style methods for imposing shear.
- Codes use standardized XML formats for parametrization and data output.
- Codes use standardized formats VTK for continuum fields and microstructures.

MANGO - Modeling Software:

- Java-based Graphical User Interface (GUI) for setting up models and simulations.
- Generates scripts and data files for SELM fluctuating hydrodynamics simulations.
- Extensible object-oriented architecture for inclusion of new SELM methods.

Available for download at: http://mango-selm.org/

MANGO-SELM Simulation Software

SELM - Simulation Software:

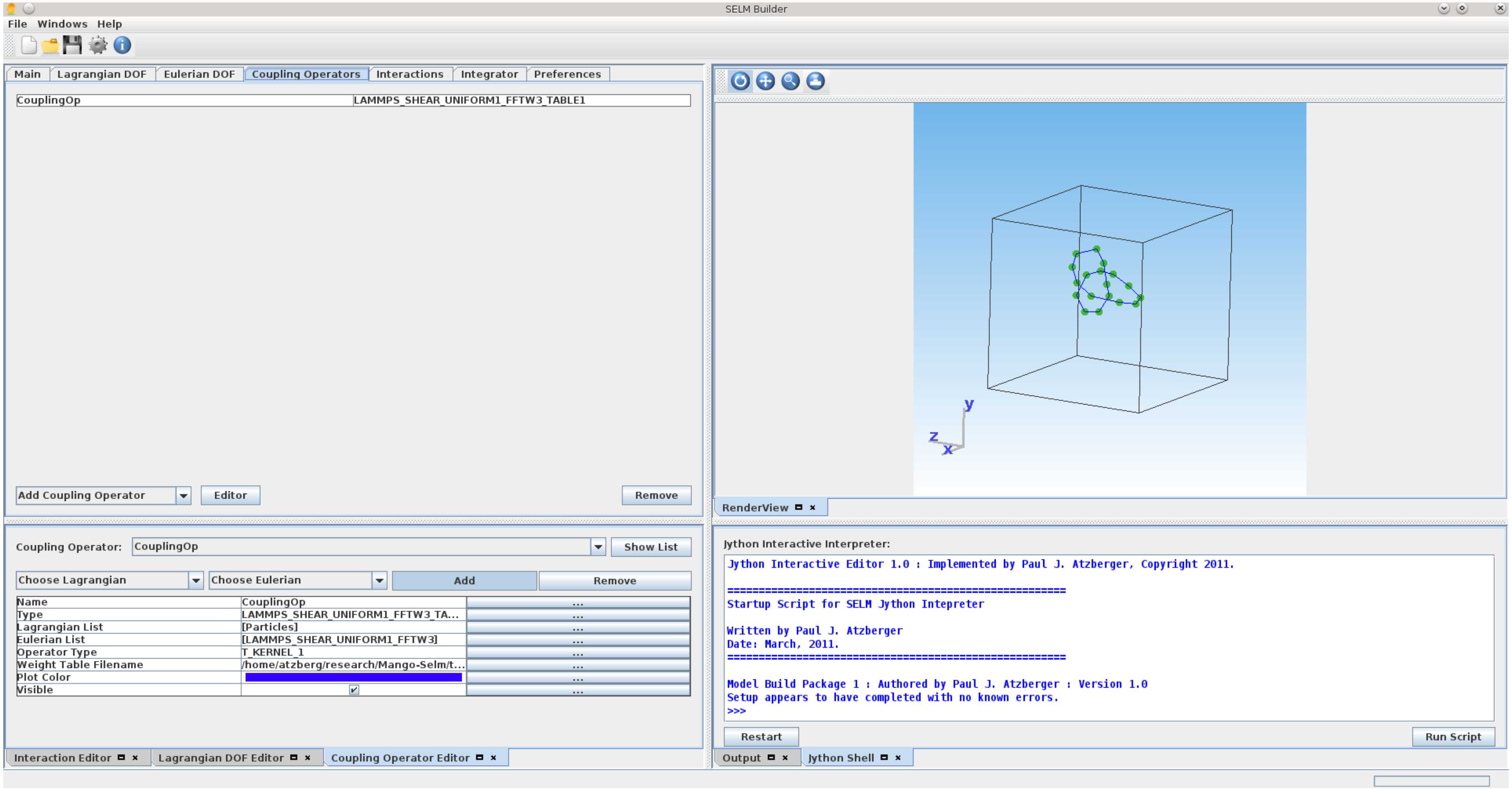
LAMMPS-SELM Interface	XML Interface
fix_SELM.cpp	Atz_XML_Helper_ParseData.cpp
fix_SELM_XML_Handler.cpp	Atz_XML_Package.cpp
SELM_Package.cpp	Atz_XML_Parser.cpp
Atz_XML_Handler_Example_A.cpp	Atz_XML_SAX_DataHandler.cpp
Atz_XML_Helper_DataHandler_List.cpp	Atz_XML_SAX_Handler_Multilevel.cpp
Atz_XML_Helper_Handler_SkipNextTag.cpp	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	

Source codes:

- C/C++ used with object-oriented classes mirroring parts of SELM
- Delegator design pattern is used to control 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.
- Codes designed to be easily extended for new types of SELM formulations and integrators.

MANGO-SELM Simulation Software

MANGO - Modeling Software:



MANGO-SELM Simulation Software

MANGO - Modeling Software:

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

MANGO-SELM Simulation Software

MANGO - Modeling Software:

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

Source codes:

- Java-based used with object-oriented classes 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
- Codes designed to be easily extended for new types of SELM formulations and integrators.
- Custom classes and interface for rendering models in 3D and interactively editing models.

MANGO-SELM Simulation Software

MANGO - Modeling Software:

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

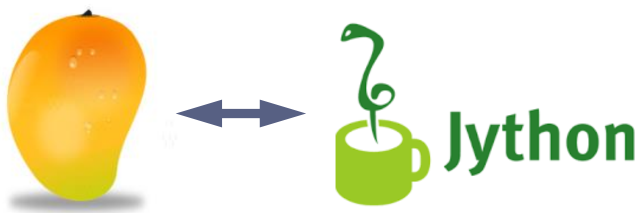
Source codes:

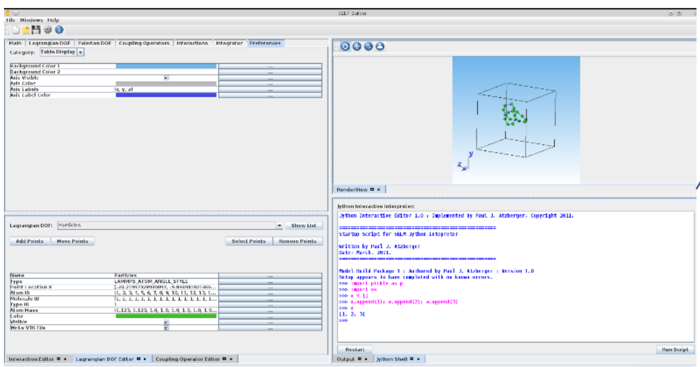
- Custom classes and interface for rendering models in 3D and interactively editing models.
- Interactive editor features allow for
    - interactive views of model
    - adding / removing control points
    - adding / removing bonds between points
    - adding custom force interactions

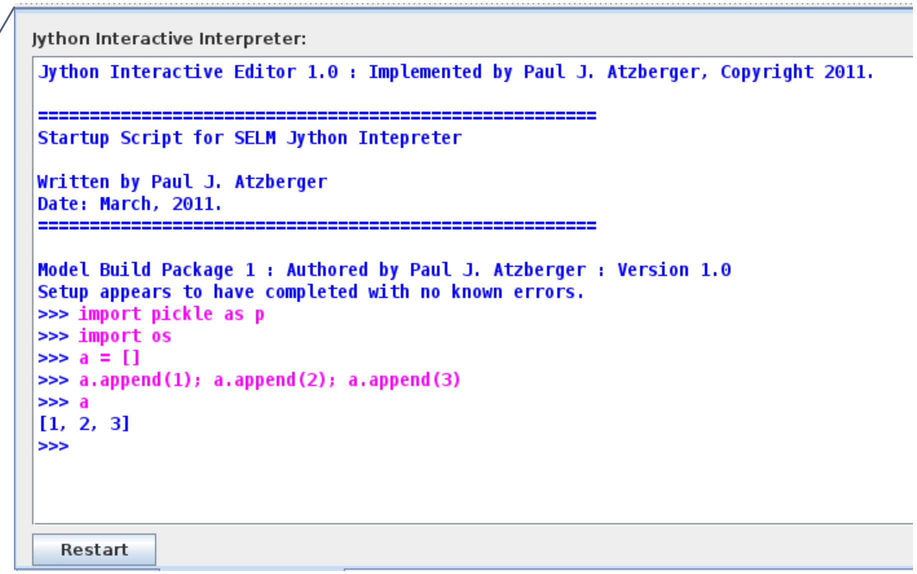
- Custom classes implemented for tracking physical units in tables.

MANGO-SELM Simulation Software

MANGO - Modeling Software:



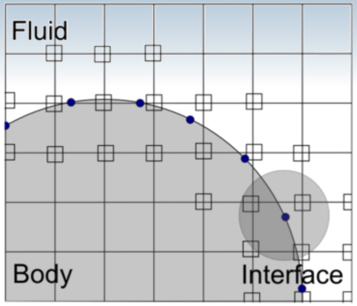




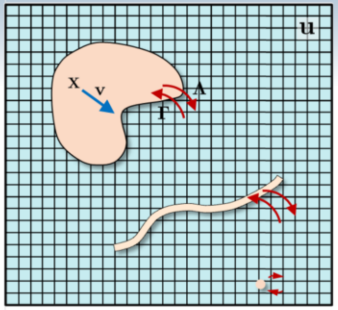
Jython Terminal:

- 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.

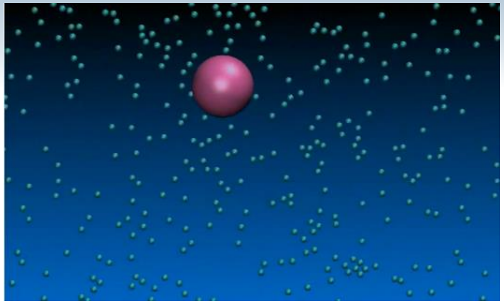
SELM Fluctuating Hydrodynamics

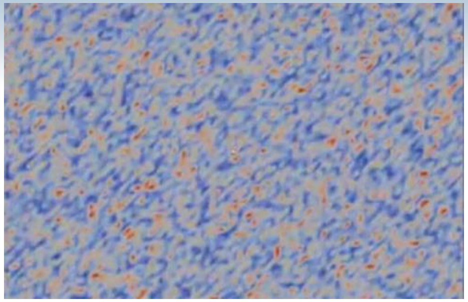


Eulerian-Lagrangian Mechanics



Eulerian-Lagrangian Coupling


Brownian Motion: Molecular Collisions


Continuum Gaussian Random Field

SELM Inertial Regime I:

hydrodynamics

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

microstructure

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}$$
$$m \frac{d\mathbf{v}}{dt} = -\Upsilon(\mathbf{v} - \Gamma \mathbf{u}) - \nabla_X \Phi[X] + \mathbf{F}_{thm}.$$

thermal fluctuations

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

SELM Overdamped Regime IV:

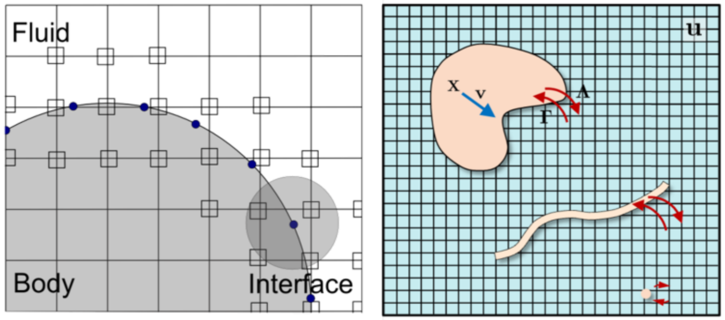
microstructure + hydrodynamics (quasi-steady)

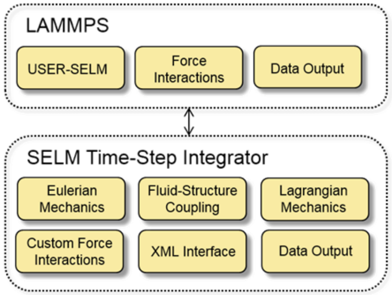
$$\frac{d\mathbf{X}}{dt} = H_{\mathrm{SELM}}[-\nabla_{\mathbf{X}} \Phi(\mathbf{X})] + (\nabla_{\mathbf{X}} \cdot H_{\mathrm{SELM}}) k_B T + \mathbf{h}_{\mathrm{thm}}$$
$$H_{\mathrm{SELM}} = \Gamma(-\wp \mathcal{L})^{-1} \Lambda$$

thermal fluctuations

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

MANGO-SELM Simulation Software





SELM Inertial Regime I (Verlet-stye temporal integration):

microstructure

$$\begin{aligned}
\mathbf{v}^{n+\frac{1}{2}} &= \mathbf{v}^{n} + \frac{\Delta t}{2} m^{-1}\mathbf{F}^{n} \\
&+ \frac{\Delta t}{2}\left(-m^{-1}\Upsilon\left(\mathbf{v}^{n-\frac{1}{2}} - \Gamma^{n}\mathbf{u}^{n-\frac{1}{2}}\right)\right. \\
&\left. + m^{-1}\mathbf{g}^{n-\frac{1}{2}}\right) \\
\mathbf{X}^{n+1} &= \mathbf{X}^{n} + \mathbf{v}^{n+\frac{1}{2}}\Delta t
\end{aligned}$$

hydrodynamics

$$\begin{aligned}
\mathbf{u}^{n+\frac{1}{2}} &= \mathbf{u}^{n} + \frac{\Delta t}{2}\rho^{-1}\mu L\mathbf{u}^{n-\frac{1}{2}} \\
&- \frac{\Delta t}{2}\left(\rho^{-1}\Lambda^{n}\left[-\Upsilon\left(\mathbf{v}^{n-\frac{1}{2}} - \Gamma^{n}\mathbf{u}^{n-\frac{1}{2}}\right)\right.\right. \\
&\left.\left. +\mathbf{g}^{n-\frac{1}{2}}\right]\right) \\
&+ \mathbf{h}^{n-\frac{1}{2}}
\end{aligned}$$

thermal fluctuations

$$\begin{aligned}
\langle \mathbf{g}^{n-\frac{1}{2}}\mathbf{g}^{n-\frac{1}{2}T}\rangle &= 4k_B T\Upsilon/\Delta t \\
\langle \mathbf{h}^{n}\mathbf{h}^{nT}\rangle &= 4k_B T\rho^{-2}\mu L/\Delta t.
\end{aligned}$$

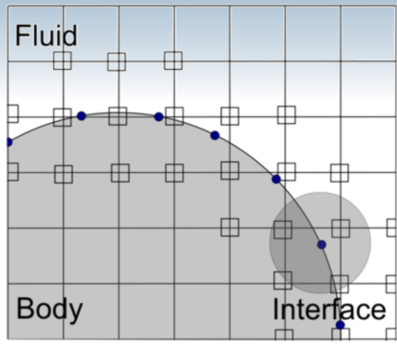
microstructure

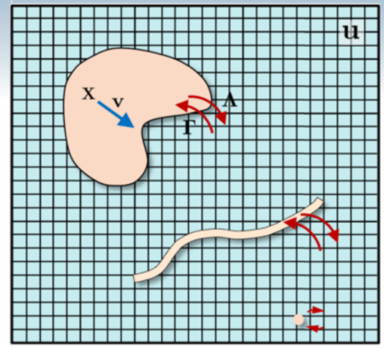
$$\begin{aligned}
\mathbf{v}^{n+1} &= \mathbf{v}^{n+\frac{1}{2}} + \frac{\Delta t}{2} m^{-1}\mathbf{F}^{n+1} \\
&+ \frac{\Delta t}{2}\left(-m^{-1}\Upsilon\left(\mathbf{v}^{n+\frac{1}{2}} - \Gamma^{n+1}\mathbf{u}^{n+\frac{1}{2}}\right)\right. \\
&\left. +m^{-1}\mathbf{g}^{n+\frac{1}{2}}\right)
\end{aligned}$$

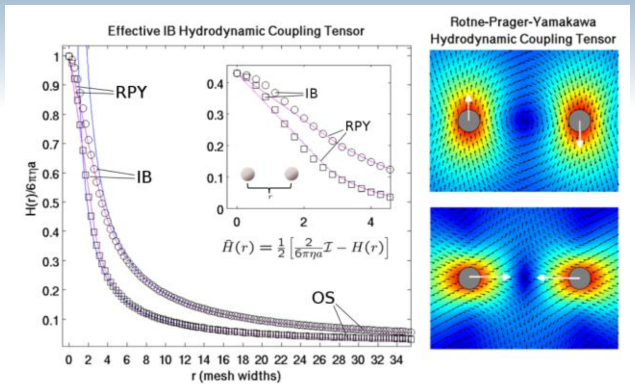
hydrodynamics

$$\begin{aligned}
\mathbf{u}^{n+1} &= \mathbf{u}^{n+\frac{1}{2}} + \frac{\Delta t}{2}\rho^{-1}\mu L\mathbf{u}^{n+\frac{1}{2}} \\
&- \frac{\Delta t}{2}\left(\rho^{-1}\Lambda^{n+1}\left[-\Upsilon\left(\mathbf{v}^{n+\frac{1}{2}} - \Gamma^{n+1}\mathbf{u}^{n+\frac{1}{2}}\right)\right.\right. \\
&\left.\left. +\mathbf{g}^{n+\frac{1}{2}}\right]\right) \\
&+ \mathbf{h}^{n+\frac{1}{2}}.
\end{aligned}$$

MANGO-SELM Simulation Software



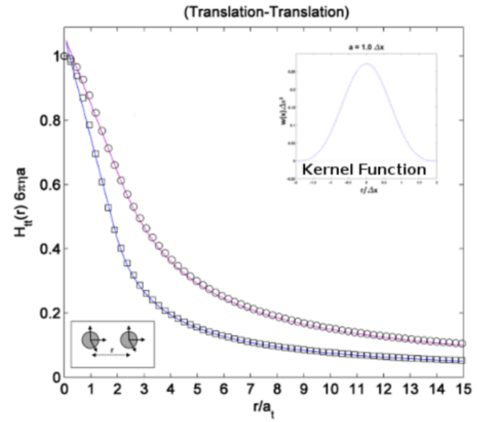




SELM Coupling:

adjoint condition

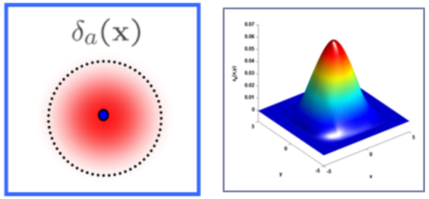
$$\langle \Gamma \mathbf{v}, \mathbf{F} \rangle = \sum_i [\Gamma \mathbf{v}]_i \cdot [\mathbf{F}]_i = \int_\Omega \mathbf{v}(\mathbf{x}) \cdot (\Lambda \mathbf{F})(\mathbf{x}) d\mathbf{x} = \langle \mathbf{v}, \Lambda \mathbf{F} \rangle$$



IB-Kernel coupling:

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

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



Peskin delta-function

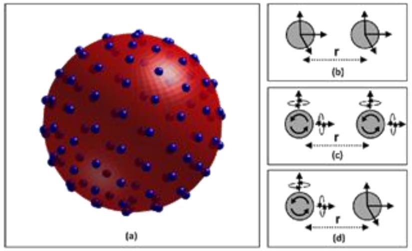
Generalized Coupling (Faxen)

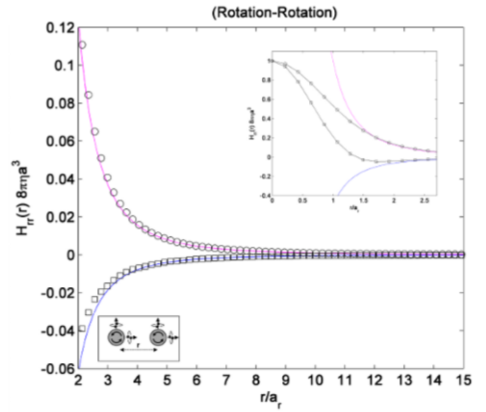
$$\Gamma_0 \mathbf{u} = \sum_{\mathbf{m}} \langle\, \eta_0(\mathbf{y_m} - (\mathbf{X}_{cm} + \mathbf{z}))\, \mathbf{u_m} \,\rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \Delta x_{\mathbf{m}}^3$$

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

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

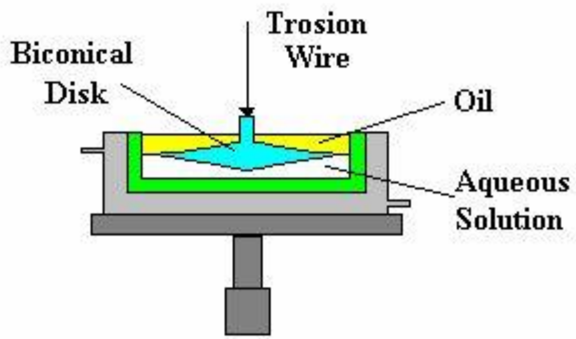
$$\Lambda_1(\mathbf{x_m}) = -\frac{3}{2R^2} \left(\langle\, \mathbf{z} \eta_1(\mathbf{x_m} - (\mathbf{X}_{cm} + \mathbf{z})) \,\rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \right) \times \mathbf{T}.$$

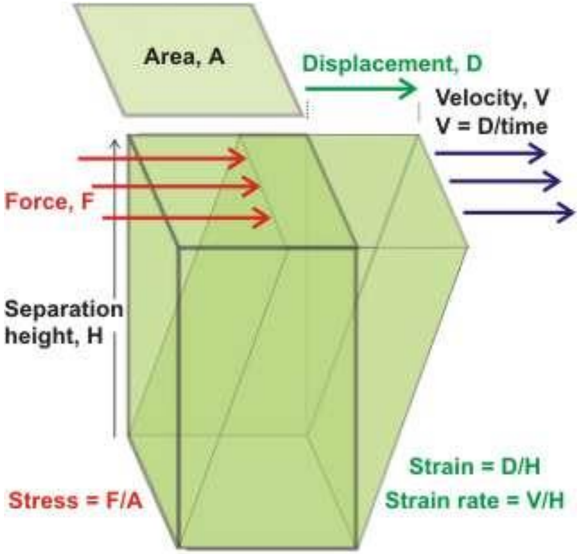




Rheological Properties and Microstructure Dynamics

Rheomety Device





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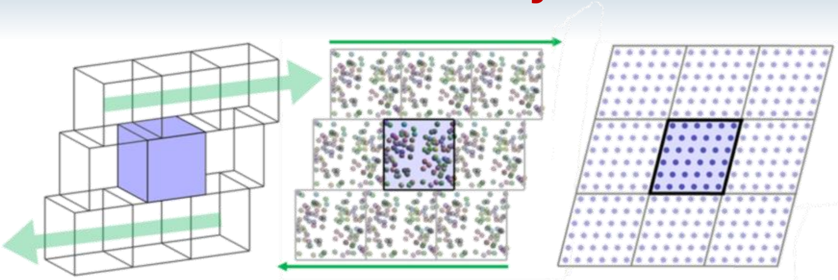
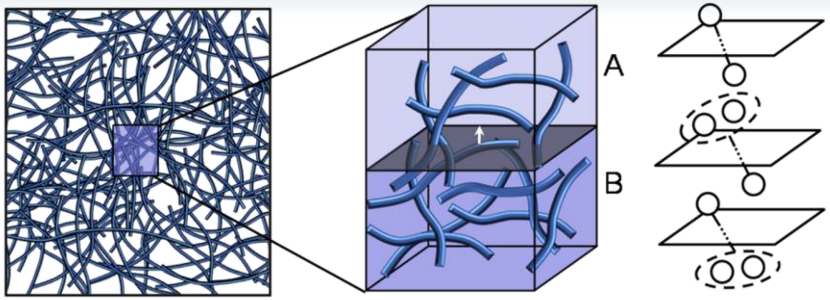
Lees-Edwards Boundary Conditions:



Material Stress ← Microscopic Forces



Stress Tensor Estimator:

$$\sigma_{\ell,z}^{(n)} = \frac{1}{AL}\sum_{\mathbf{q}\in\mathcal{Q}_n}\sum_{j=1}^{n-1}\left\langle \mathbf{f}_{\mathbf{q},j}^{(\ell)}\cdot\left(\mathbf{x}_{q_n}^{*,(z)} - \mathbf{x}_{q_j}^{*,(z)}\right)\right\rangle$$

Fluctuating hydrodynamics (moving frame):

$$\rho\frac{d\mathbf{w}}{dt} = L(t)\mathbf{w} + \lambda + \Lambda[-\nabla_{\mathbf{X}}\Phi] + (\nabla_{\mathbf{X}}\cdot\Lambda)\,k_B T + \mathbf{J} + \mathbf{h}_{\mathrm{thm}}$$

$$S(t)\cdot\mathbf{w} = \mathbf{K}$$

$$\frac{d\mathbf{X}}{dt} = \Gamma\mathbf{w}.$$

$$S(t)\cdot\mathbf{w} = D\cdot\mathbf{w} + \mathbf{e}_z^T\; G\mathbf{w}\;\mathbf{e}_x\dot{\gamma}t$$

$$L(t)\mathbf{w} = \mu\left[\mathbf{e}_d - \delta_{d,3}\dot{\gamma}t\mathbf{e}_x\right]^T A\mathbf{w}\left[\mathbf{e}_d - \delta_{d,3}\dot{\gamma}t\mathbf{e}_x\right]$$

$$G(s,t) = \langle\mathbf{h}_{\mathrm{thm}}(s)\mathbf{h}_{\mathrm{thm}}(t)^T\rangle$$

$$G(s,t) = -2\wp(t)L(t)C\delta(t-s)$$

$$D\cdot\mathbf{w} = \sum_{d=1}^{3}\frac{\mathbf{w}^{(d)}(\mathbf{q}+\mathbf{e}_d) - \mathbf{w}^{(d)}(\mathbf{q}-\mathbf{e}_d)}{2\Delta x}$$

$$[G\mathbf{w}]_{ij} = \frac{\mathbf{w}^{(i)}(\mathbf{q}+\mathbf{e}_j) - \mathbf{w}^{(i)}(\mathbf{q}-\mathbf{e}_j)}{2\Delta x}$$

$$[A\mathbf{w}]_{ii} = \frac{\mathbf{w}^{(i)}(\mathbf{q}+\mathbf{e}_i) - 2\mathbf{w}^{(i)}(\mathbf{q}) + \mathbf{w}^{(i)}(\mathbf{q}-\mathbf{e}_i)}{\Delta x^2}$$

$$[A\mathbf{w}]_{ij} = \frac{\mathbf{w}^{(d)}(\mathbf{q}+\mathbf{e}_i+\mathbf{e}_j) - \mathbf{w}^{(d)}(\mathbf{q}-\mathbf{e}_i+\mathbf{e}_j)}{4\Delta x^2} - \frac{\mathbf{w}^{(d)}(\mathbf{q}+\mathbf{e}_i-\mathbf{e}_j) - \mathbf{w}^{(d)}(\mathbf{q}-\mathbf{e}_i-\mathbf{e}_j)}{4\Delta x^2},\; i\neq j.$$

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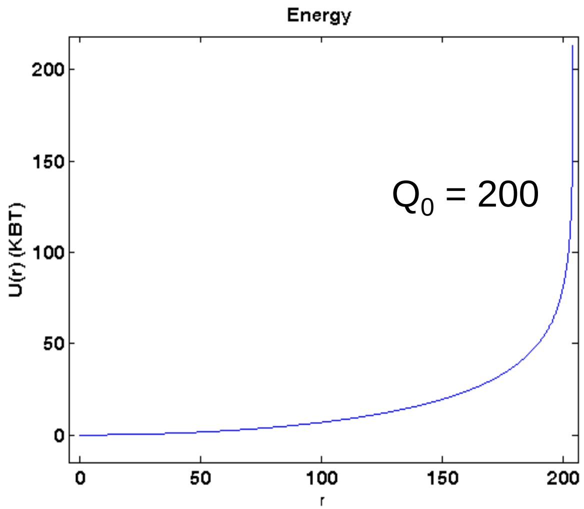
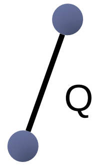
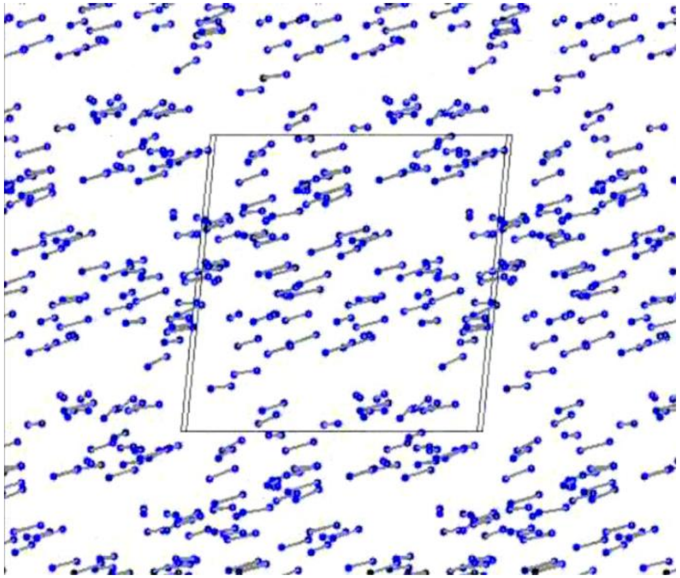
Example System : Finitely Extensible Nonlinear Elastic (FENE) Dimers:

Potential Energy:

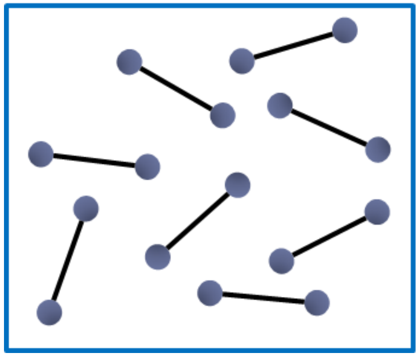
$$U(r) = -\frac{K}{2}Q_0^2 \log(1 - (Q/Q_0)^2)$$



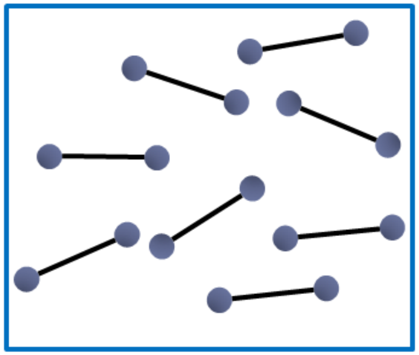




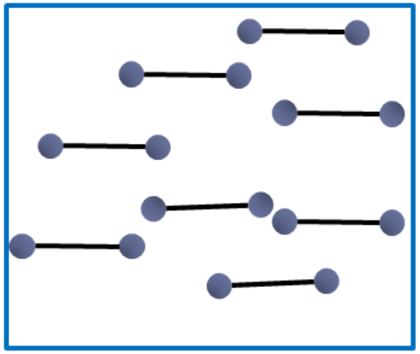
low shear rate



medium shear rate

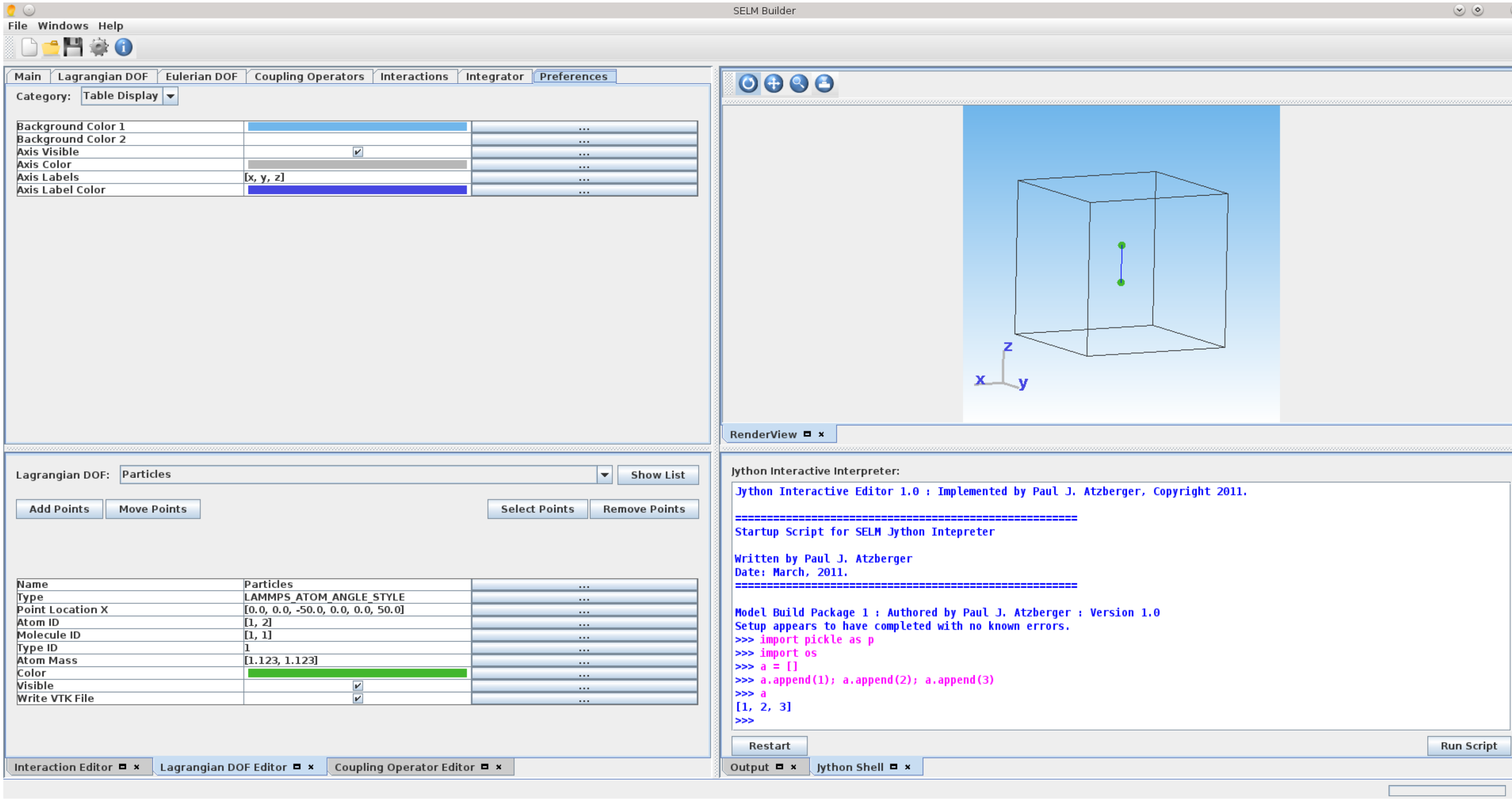


large shear rate



MANGO-SELM Simulation Software

MANGO - Modeling Software:



MANGO-SELM Simulation Software

MANGO-SELM – Download: http://mango-selm.org/

Mango-Selm | Fluctuating Hydrodynamics

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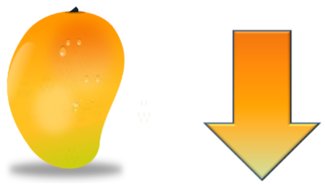


Downloads

Please join our mailing list for the announcement of updated releases.

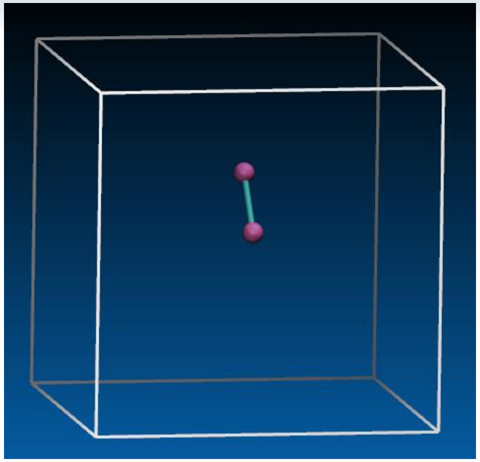
- Download Latest Release

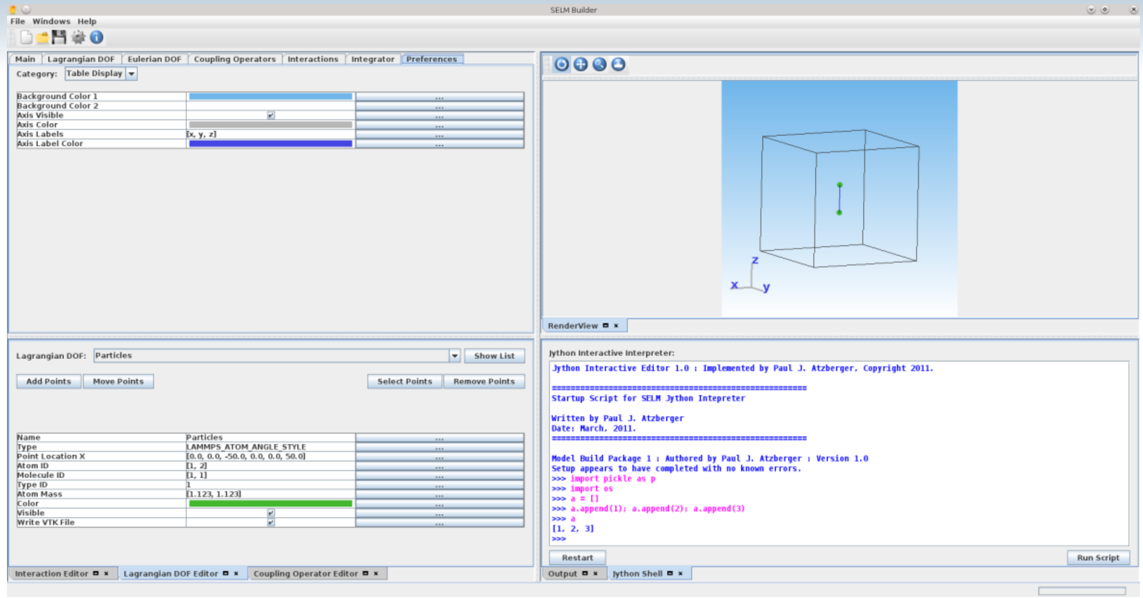
Additional Information

- Installation Instructions
- Tutorials for Setting up Simulations
- Mango-Selm Announcements
- Mango-Selm Discussion Forum
- Mango-Selm Issue Tracker

MANGO-SELM Simulation Software

Demo Live: FENE_Dimer





Steps:

1. Use File→Open project.

2. Load: Fene_Dimer/FeneModel.SELM_Builder_Project

3. Adjust coupling operator table to /common/CouplingOp_T_KERNEL_1.SELM_CouplingOperator_weightTable

4. Gear Icon → generate SELM simulation files.

5. Link executable in ln –s …./common/ SELM_LAMMPS_serial_x86_Ubuntu run

6. run –in Fene_Dimer.LAMMPS_script

7. Generates output data → .dcd file.

8. Run ./vis_FENE.vmd to visualize the model.

Important files:

FENE_Dimer.LAMMPS_script
FENE_Dimer.LAMMPS_read_data
FENE_Dimer.SELM_Info
FENE_Dimer.SELM_InfoExtra
FENE_Dimer.SELM_params
FENE-bonds.SELM_Interaction

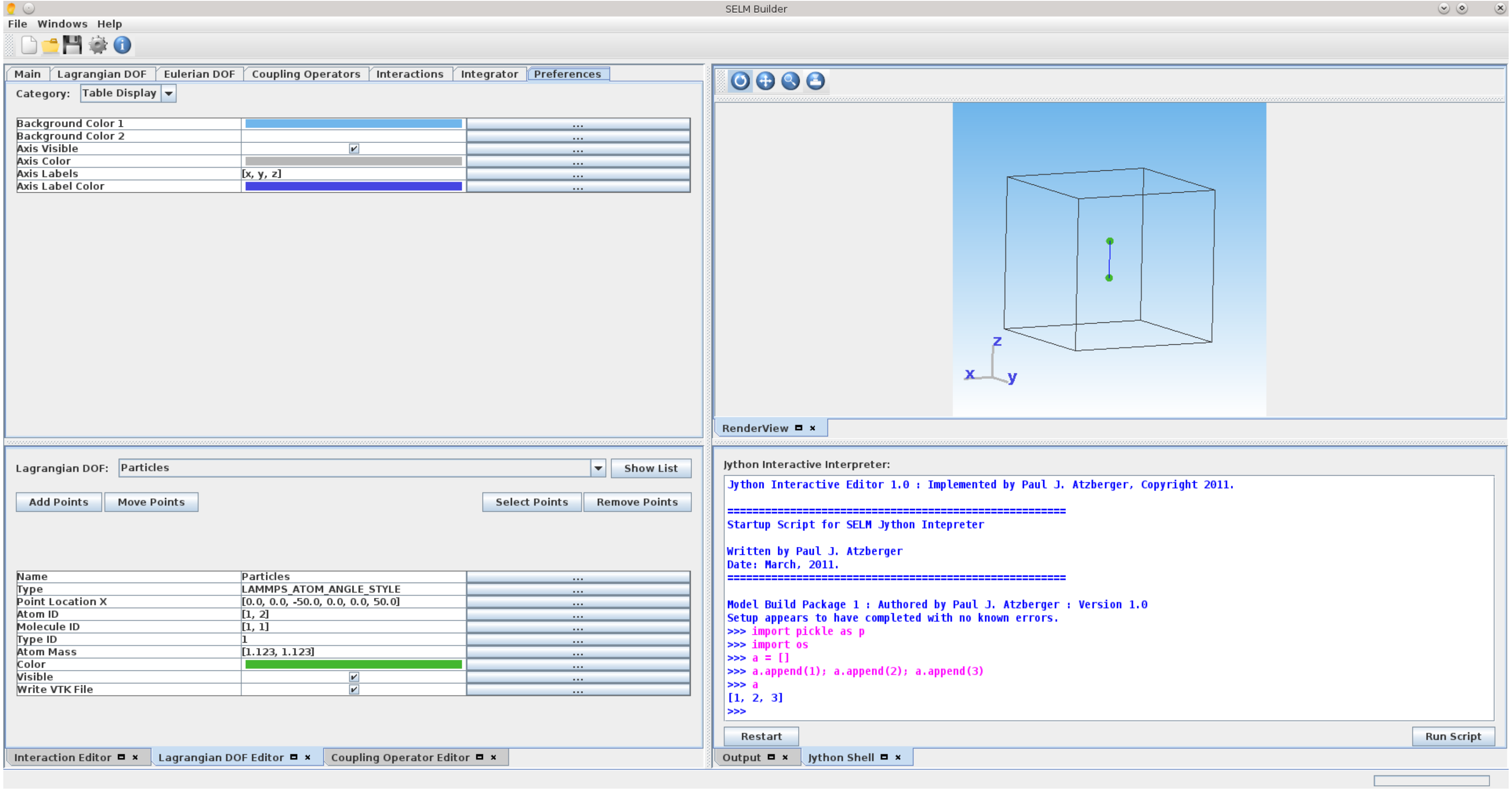
CouplingOp.SELM_CouplingOperator
CouplingOp_T_KERNEL_1.SELM_CouplingOperator_weightTable

LAMMPS_SHEAR_QUASI_STEADY1_FFTW3.SELM_Integrator
LAMMPS_SHEAR_UNIFORM1_FFTW3.SELM_Eulerian
Particles.SELM_Lagrangian

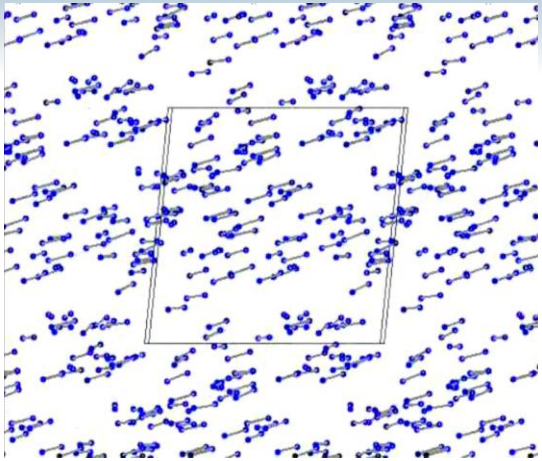
SELM_LAMMPS_serial_x86_Ubuntu
*.dcd
vis1.vmd

MANGO-SELM Simulation Software

Demo Live: FENE

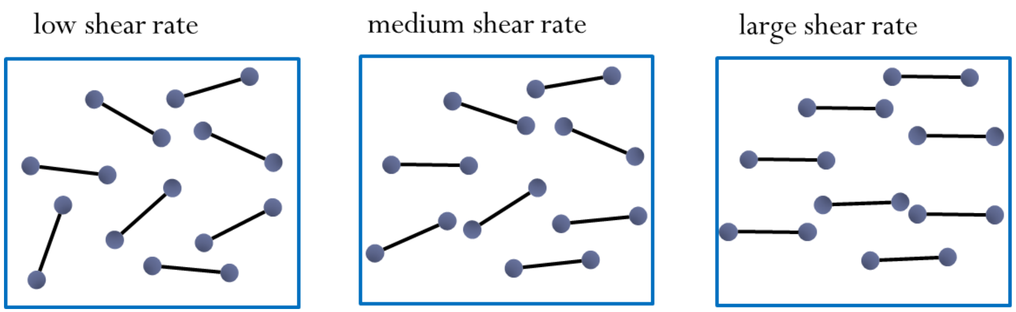


MANGO-SELM Simulation Software

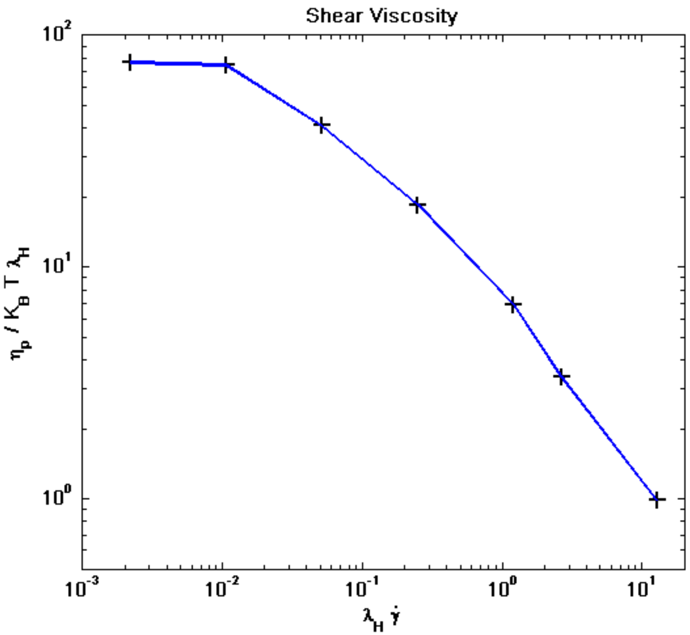


Finitely Extensible Nonlinear Elastic (FENE) Dimers:

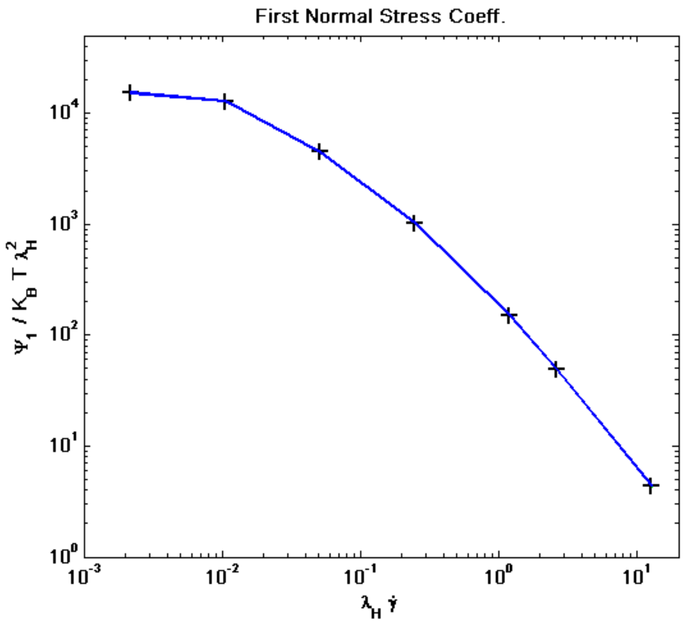
$$U(r) = -\frac{K}{2}Q_0^2 \log(1 - (Q/Q_0)^2)$$



Shear Viscosity $\eta_p = \frac{\sigma^{(s,v)}}{\dot{\gamma}}$

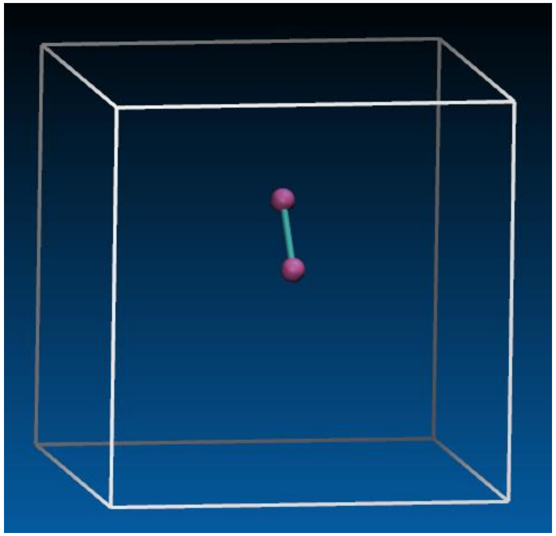


First Normal Stress $\Psi_1 = \frac{\sigma^{(s,s)} - \sigma^{(v,v)}}{\dot{\gamma}^2}$

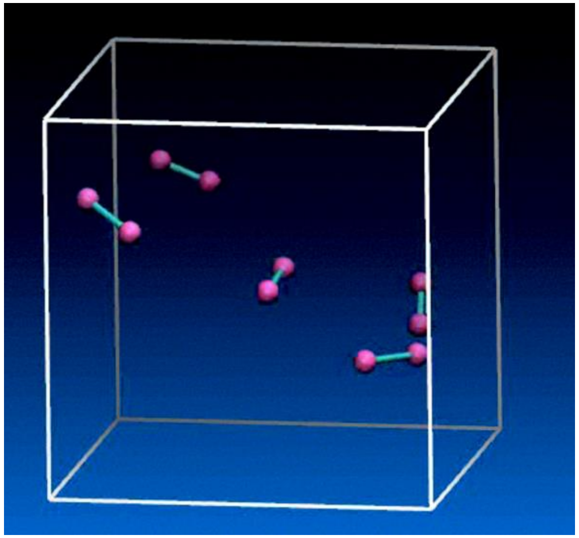


MANGO-SELM Simulation Software

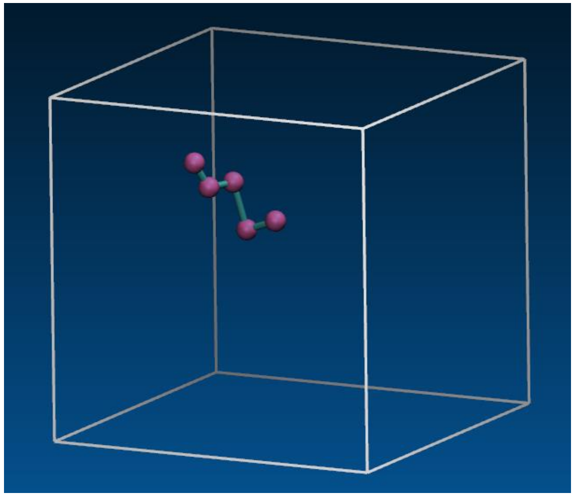
Other Demos:



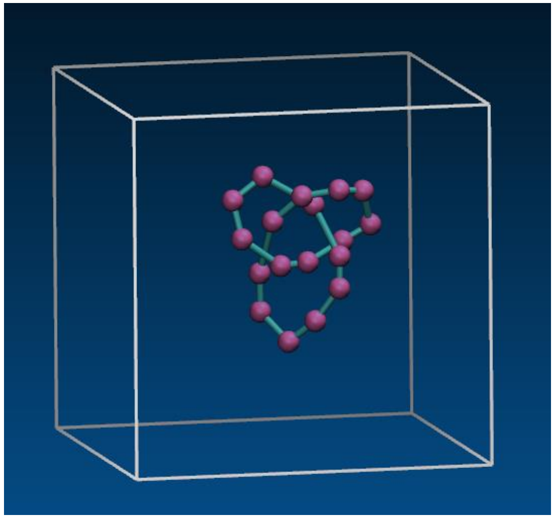
Sheared FENE Dimer



FENE Fluid



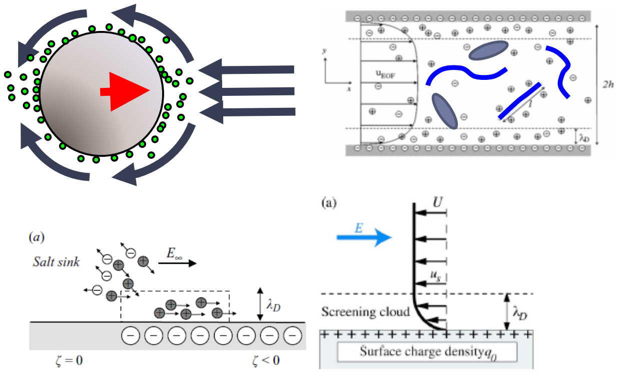
Polymer Chain



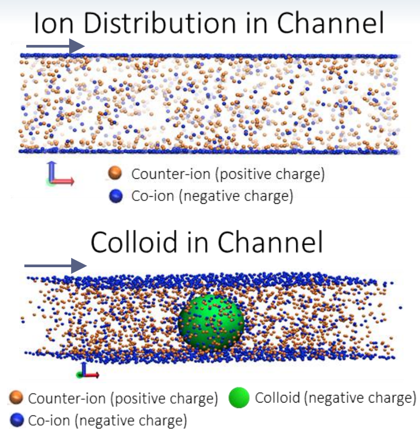
Polymer Knot

Fluidics Transport

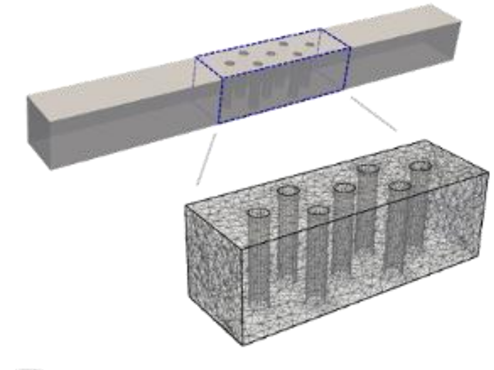
Fluidic Devices



Electrokinetics



Geometry / Confinement



Fluidic Devices

- Developed to miniaturize and automate many laboratory tests, diagnostics, characterization.
- Hydrodynamic transport at such scales must grapple with dissipation / friction.
- Electrokinetic effects utilized to drive flow.

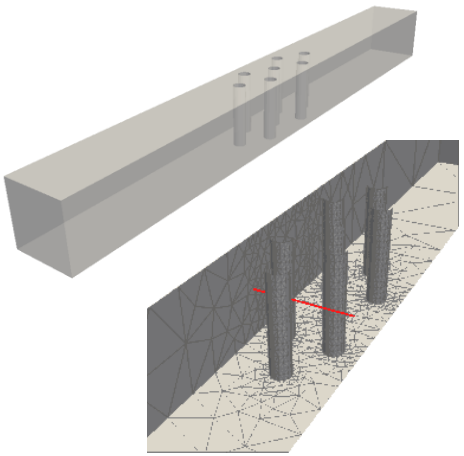
Key Features

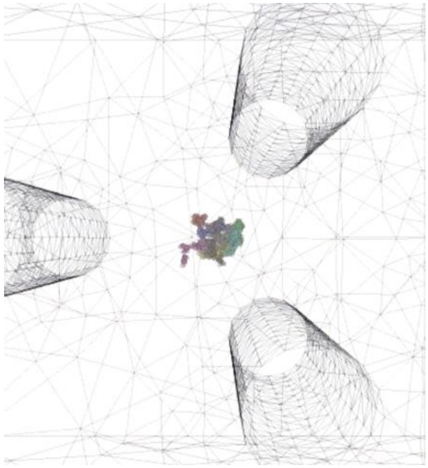
- Large surface area to volume.
- Ionic double-layers can be comparable to channel width.
- Brownian motion plays important role in ion distribution and analyte diffusion across channel.
- Hydrodynamic flow effected by close proximity to walls or other geometric features.
- Ionic concentrations often in regime with significant discrete correlations /density fluctuations.

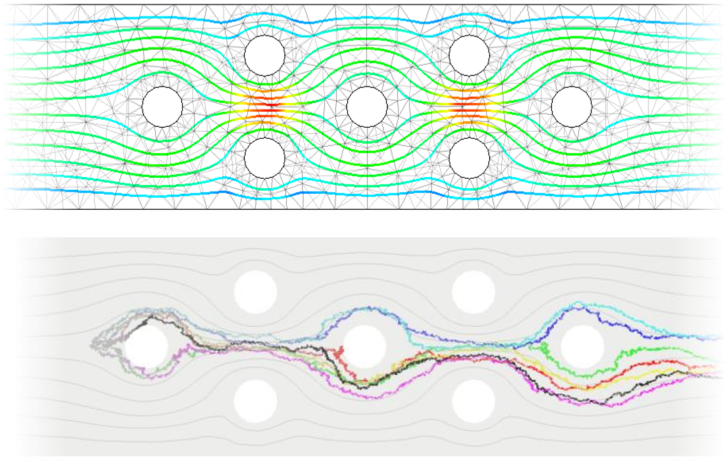
Challenges

- Develop theory and methods beyond mean-field Poisson-Boltzmann theory.
- Methods capable of handling hydrodynamics, fluctuations, geometry/confinement.

Mesoscale Simulations : Fluidics Channel



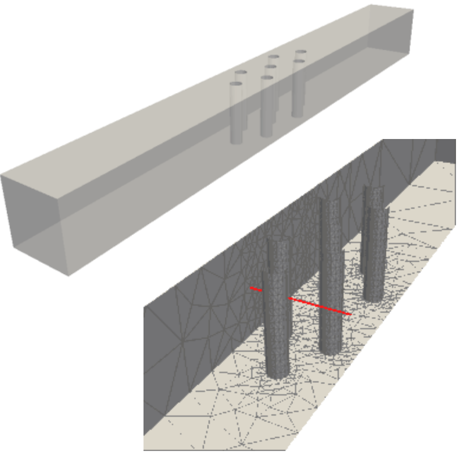


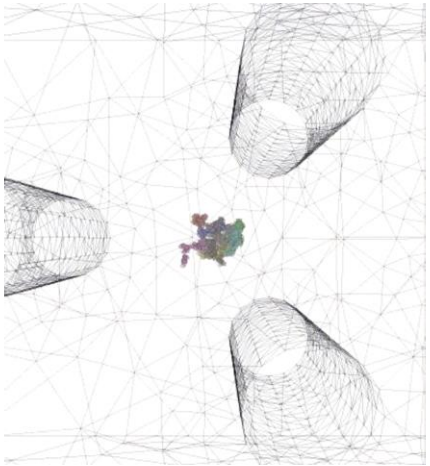


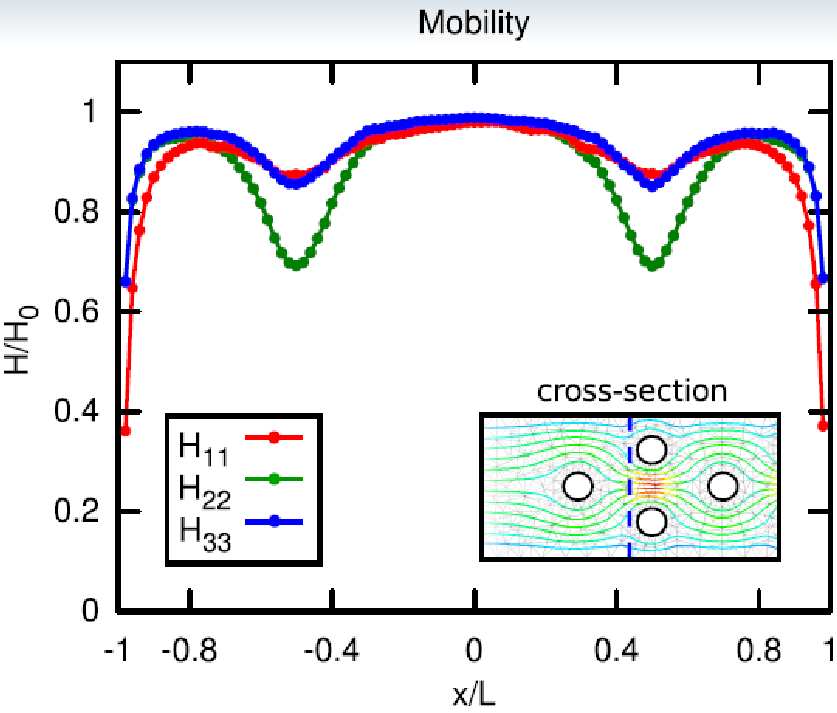
Considerations:

- FEM-SELM approach used to study advection-diffusion in microfluidic device geometry.
- Particle interactions with walls and post-obstacles (gel-free electrophoresis / sorting).
- Hydrodynamic responses and diffusivity augmented by proximity to walls / obstacles.

Mesoscale Simulations : Fluidics Channel





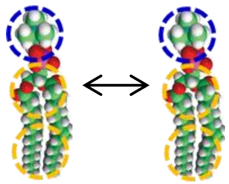


Considerations:

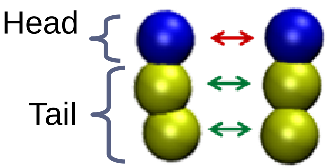
- FEM-SELM approach used to study advection-diffusion in microfluidic device geometry.
- Particle interactions with walls and post-obstacles (gel-free electrophoresis / sorting).
- Hydrodynamic responses and diffusivity augmented by proximity to walls / obstacles.

Coarse-Grained Lipid Model

Lipid Interactions



Coarse-Grained Model



Deserno 2005.

Interaction Potentials

Steric Repulsion: Weeks-Chandler Anderson

$$V_{\text{steric}}(r) = \begin{cases} 4\epsilon\left[(b/r)^{12} - (b/r)^6 + 1/4\right], & r \leq r_c, \\ 0, & r > r_c. \end{cases} \quad r_c = 2^{1/6}b$$

Bonds: FENE

$$V_{\text{bond}}(r) = -\frac{1}{2}k_{\text{bond}}r_\infty^2 \ln\left(1 - (r/r_\infty^2)\right)$$

Bending

$$V_{\text{bend}}(r) = \frac{1}{2}k_{\text{bend}}\left(r - 4\sigma\right)^2$$

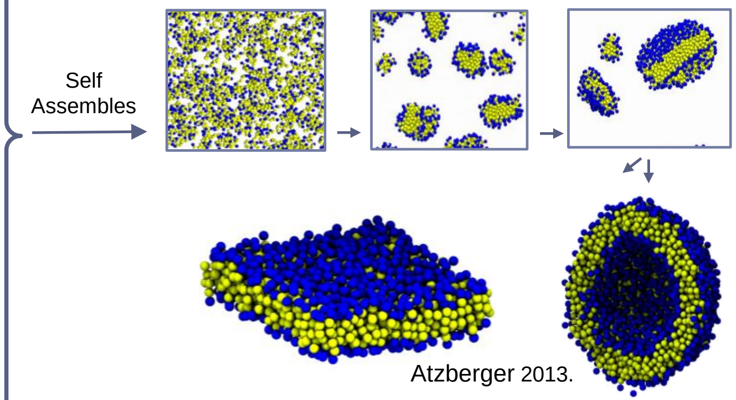
Tail-Tail Attraction: Hydrophobic-Hydrophilic Effect

$$V_{\text{tail-tail}}(r) = \begin{cases} -\epsilon, & r < r_c, \\ -\epsilon\cos^2(\pi(r - r_c)/2w_c), & r_c \leq r \leq r_c + w_c, \\ 0, & r > r_c. \end{cases}$$

Deserno 2005.

Lipid Bilayer Membranes

Self-Assembled Bilayers

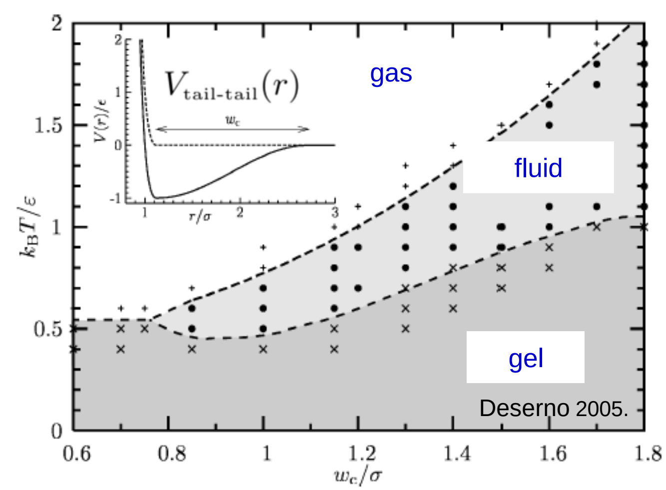


Atzberger 2013.

Key Features

- Atomic details coarse-grained to obtain simplified model.
- Lipids represented by a few "beads."
- Hydrophobic-hydrophilic effect drives bilayer formation.
- Solvent treated implicitly through free energy of interactions.
- Long-range tail-tail interaction drives self-assembly (important to obtain fluid phase).
- IS-CG models widely used for equilibrium. What about kinetics?

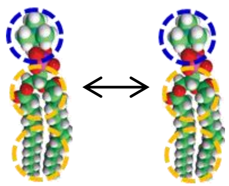
Phases



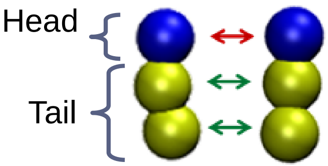
Deserno 2005.

Extending IS-CG Models with Fluctuating Hydrodynamics

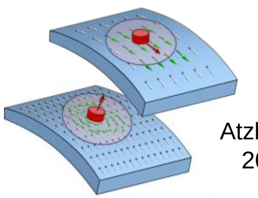
Lipid Interactions



Coarse-Grained Model



Deserno 2005.



Atzberger 2016.

Fluctuating Hydrodynamics

Particle Dynamics:

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}$$

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

Fluctuating Hydrodynamics (SELM):

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

$$\nabla \cdot \mathbf{u} = 0.$$

Thermal Fluctuations

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

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

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

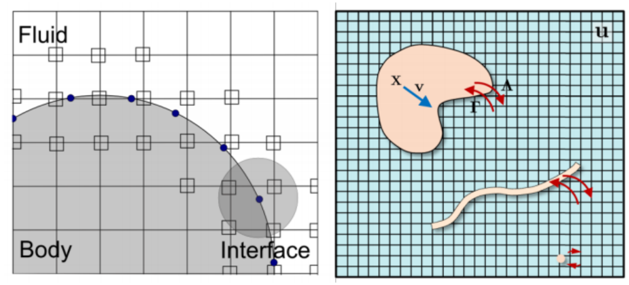
Coupling by Immersed Boundary Method

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

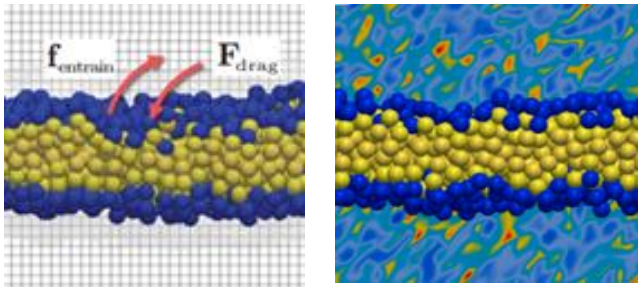
$$\Lambda\mathbf{F} = \eta\left(\mathbf{x} - \mathbf{X}(t)\right)\mathbf{F}.$$

Atzberger 2007

Stochastic Eulerian-Lagrangian Method



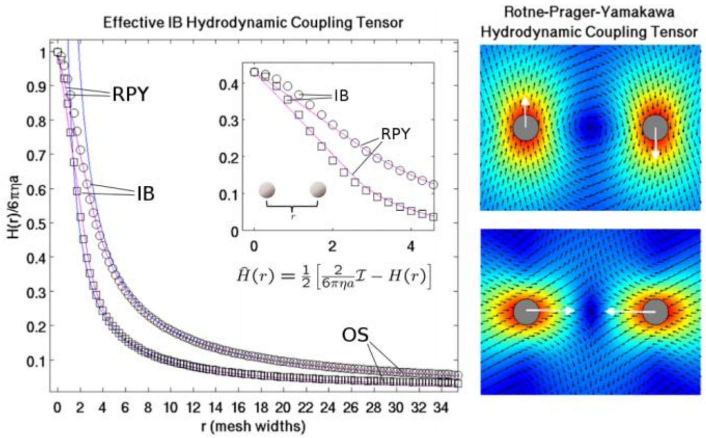
SELM-CG Bilayer Model



Extending Implicit Solvent Models for Kinetics

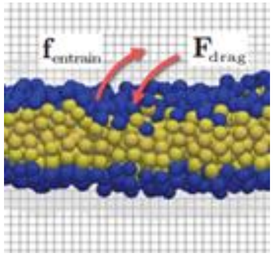
- Solvent treated implicitly (free energy contributions).
- Missing momentum transport through solvent.
- Saffman-Delbruck diffusion shows solvent important!
- We introduce fluctuating hydrodynamics to thermostat system.
- Extends IS-CG models for kinetic studies (SELM-CG).

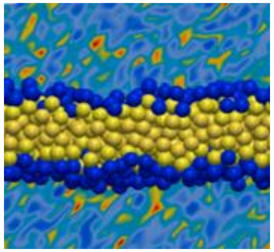
Hydrodynamic Coupling



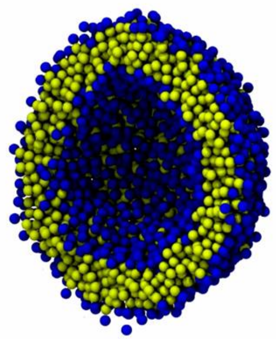
SELM-CG Bilayer Model

SELM-CG Bilayer Model



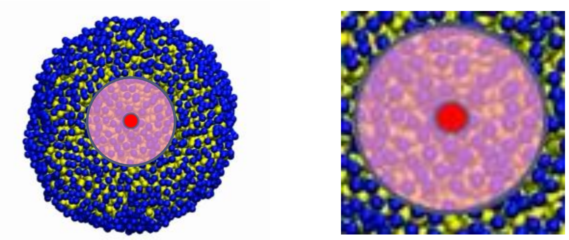


Lipid Vesicles

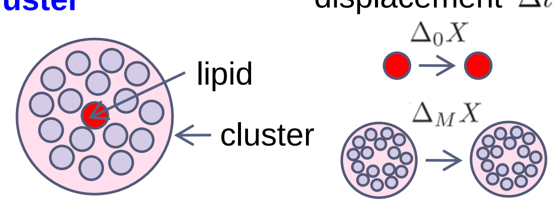


Correlation Analysis

Lipid Vesicle



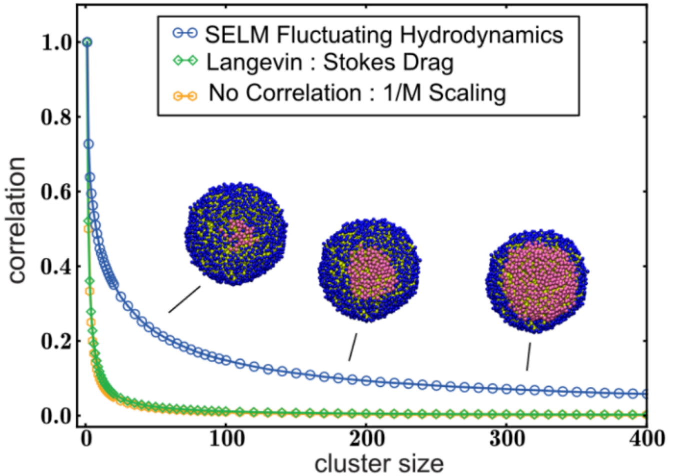
Cluster



Cluster Correlation: Dynamics

$$c_M = \langle \Delta_0 X \Delta_M X \rangle / \langle \Delta_0 X^2 \rangle$$

Results: SELM vs Langevin Stokes



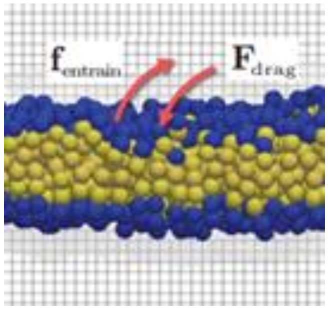
Lipid Dynamics within Vesicle Bilayers

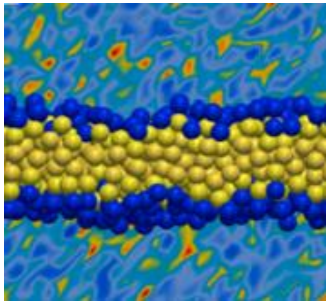
- Saffman-Delbruck diffusion shows solvent is important!
- Lipid motions correlated through direct contacts and solvent flow.
- Langevin dynamics models momentum transfer as local.
- Lipid dynamics: consider correlations within a cluster.
- SELM-CG vs Langevin dynamics (Stokes drag).
- Langevin drag suppresses lateral correlations.
- SELM exhibits long-range correlations.

Atzberger 2013

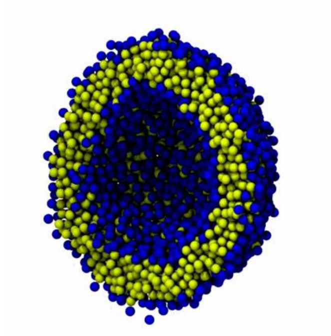
SELM-CG Bilayer Model

SELM-CG Bilayer Model



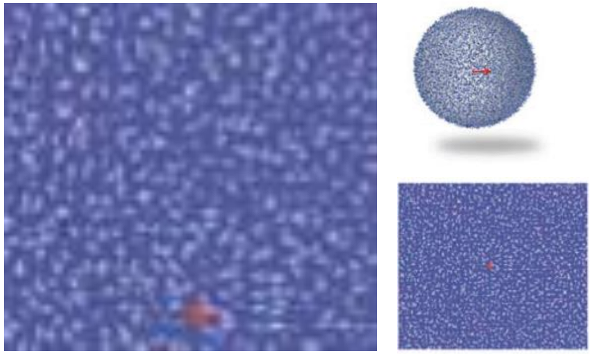


Lipid Vesicles



Results

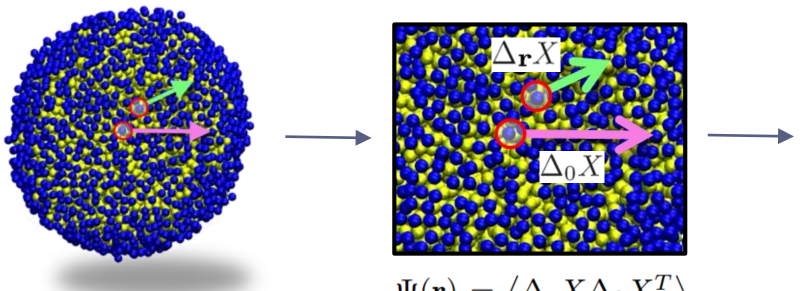
Langevin:Stokes Drag



Correlation Analysis

Two-point correlation

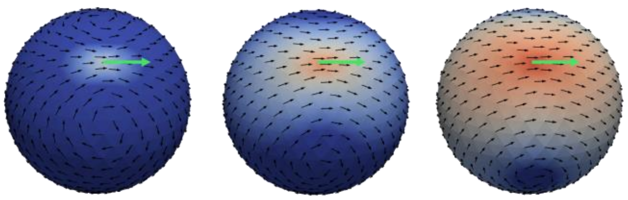
Displacement Δt



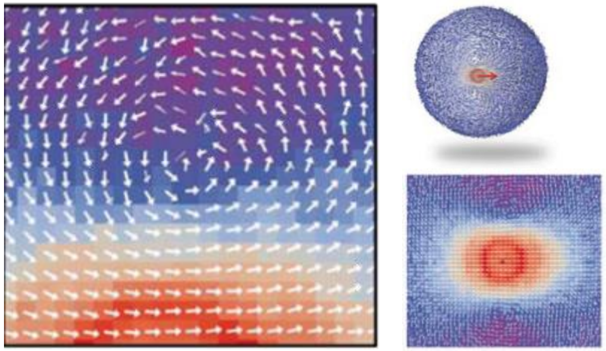
$$\Psi(\mathbf{r}) = \langle \Delta_{\mathbf{r}} X \Delta_0 X^T \rangle$$

Spatial Correlation

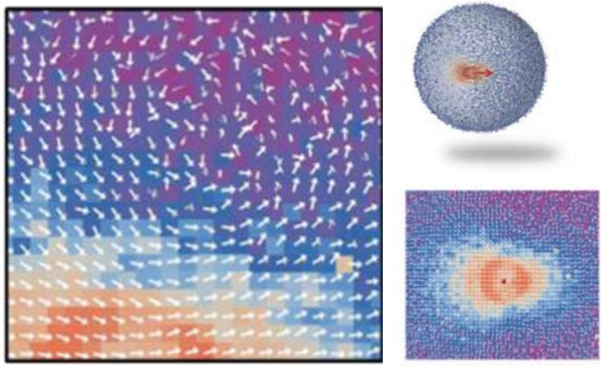
Lipid Displacement Correlations



SELM: Fluctuating Hydrodynamics



Langevin: Small Drag

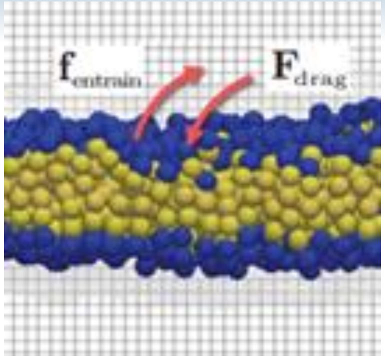


Lipid Dynamics within Vesicle Bilayers

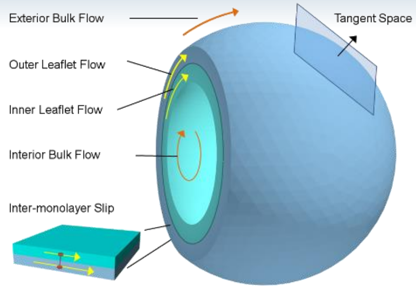
- Spatial analysis of lipid motions (passive fluctuations).
- Two point correlations (linear response to point force).
- SELM vs Langevin Dynamics.

Atzberger et al, 2013, 2016

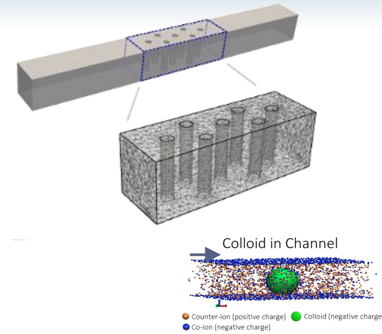
Conclusions



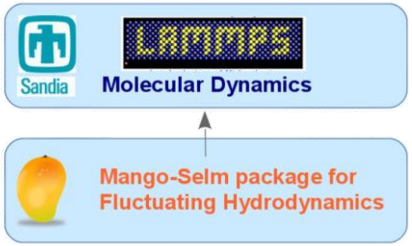
Coarse-Grained Lipid Models
Fluctuating Hydrodynamics Approaches



Continuum Mechanics of Bilayer Membranes
Fluctuating Hydrodynamics Approaches



Hybrid Descriptions for Fluidics
Fluctuating Hydrodynamics Approaches



http://mango-selm.org/

SELM Fluctuating Hydrodynamics
Software Packages

Summary

- Stochastic Eulerian Lagrangian Method (SELM) for fluctuating hydrodynamic descriptions of mesoscale systems.
- SELM incorporates into traditional hydrodynamic and CFD approaches the role of thermal fluctuations.
- Developed both coarse-grained and continuum approaches for soft-materials and fluidics.
- Many applications: polymeric fluids, colloidal systems, lipid bilayer membranes, electrokinetics, fluidics.
- Open source package in LAMMPS MD for SELM simulations: http://mango-selm.org/

Recent Students / Post-docs

- B. Gross
- J. K. Sigurdsson
- Y. Wang
- P. Plunkett
- G. Tabak
- M. Gong
- I. Sidhu

CM4 Collaborators

- C. Siefert, J. Hu, M. Parks (Sandia)
- A. Frischknecht (Sandia)
- H. Lei, G. Schenter, N. Baker (PNNL)
- N. Trask (Brown / Sandia)

Funding

- NSF CAREER
- DOE CM4
- Keck Foundation

More information: http://atzberger.org/

Publications

Hydrodynamic Coupling of Particle Inclusions Embedded in Curved Lipid Bilayer Membranes, J.K. Sigurdsson and P.J. Atzberger, (submitted), (2016) http://arxiv.org/abs/1601.06461

Fluctuating Hydrodynamics Methods for Dynamic Coarse-Grained Implicit-Solvent Simulations in LAMMPS, Y. Wang, J. K. Sigurdsson, and P.J. Atzberger, SIAM J. Sci. Comp. (accepted), (2016).

Systematic Stochastic Reduction of Inertial Fluid-Structure Interactions subject to Thermal Fluctuations, G. Tabak and P.J. Atzberger, SIAM J. Appl. Math., 75(4), 1884–1914, (2015).

Spatially Adaptive Stochastic Methods for Fluid-Structure Interactions Subject to Thermal Fluctuations in Domains with Complex Geometries, P. Plunkett, J. Hu, C. Siefert, P.J. Atzberger, Journal of Computational Physics, Vol. 277, 15 Nov. 2014, pg. 121--137, (2014).

Dynamic Implicit-Solvent Coarse-Grained Models of Lipid Bilayer Membranes : Fluctuating Hydrodynamics Thermostat, Y. Wang, J. K. Sigurdsson, E. Brandt, and P.J. Atzberger, Phys. Rev. E 88, 023301, (2013).

Incorporating Shear into Stochastic Eulerian Lagrangian Methods for Rheological Studies of Complex Fluids and Soft Materials, P.J. Atzberger, Physica D, Vol. 265, pg. 57–70, (2013).

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

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).

More information: http://atzberger.org/