Planktos: An agent-based modeling framework for collective behavior in fluid flow around immersed structures

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Small organisms in fluid around immersed structures

Laura Miller
University of Arizona

Nick Battista
The College of New Jersey

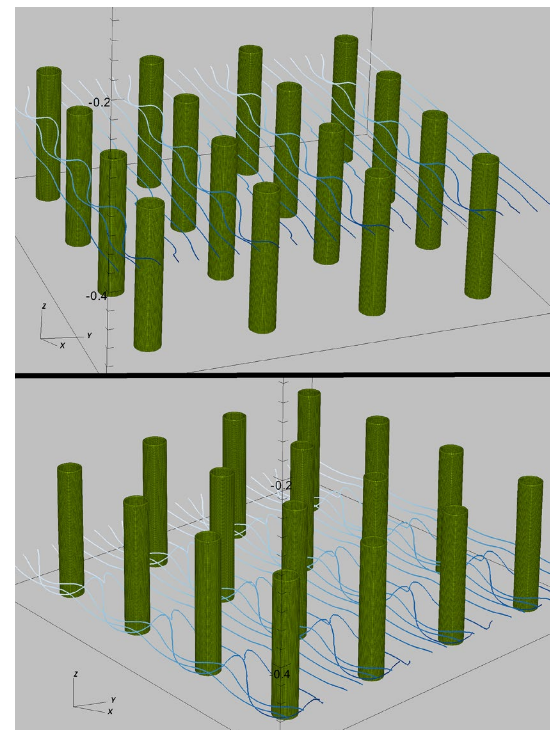
Biological motivation

The collective way in which **small organisms** interact with **immersed structures** and their **surrounding fluid flow** can be of critical ecological significance.

Biological protective layers:

The **microenvironment** created by vegetation and coral reefs supports the persistence of zooplankton, which form the foundation of the ecosystem.

Strickland, Miller, et al. (2017), “Three-Dimensional Low Reynolds Number Flows near Biological Filtering and Protective Layers”



Biological motivation

The collective way in which **small organisms** interact with **immersed structures** and their **surrounding fluid flow** can be of critical ecological significance.

Filter feeding by predators:

Organisms such as coral and jellyfish have morphology which is likely **optimized in part to increase plankton uptake**. They also actively manipulate the flow.

At the same time, plankton are known to detect disturbances in the flow, and these can trigger **escape responses**.

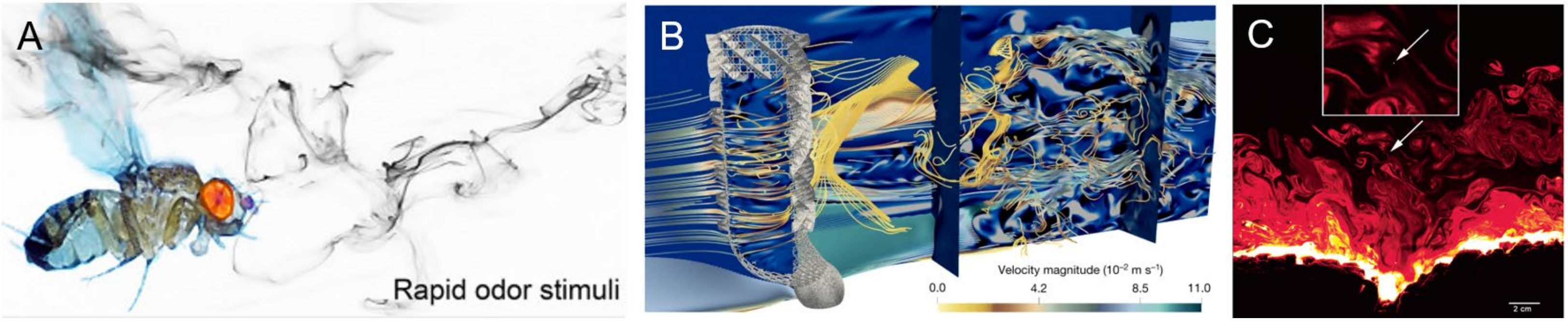
Biological motivation

The collective way in which **small organisms** interact with **immersed structures** and their **surrounding fluid flow** can be of critical ecological significance.

Small organism search strategies:

- Corals contend with the challenge of **capturing** species-specific sperm from an extremely large volume of fluid.
- Tiny parasitoid wasps must **find** equally tiny hosts (1 mm).

Chemical cues may play a role, but small organisms have limited energy to expend.



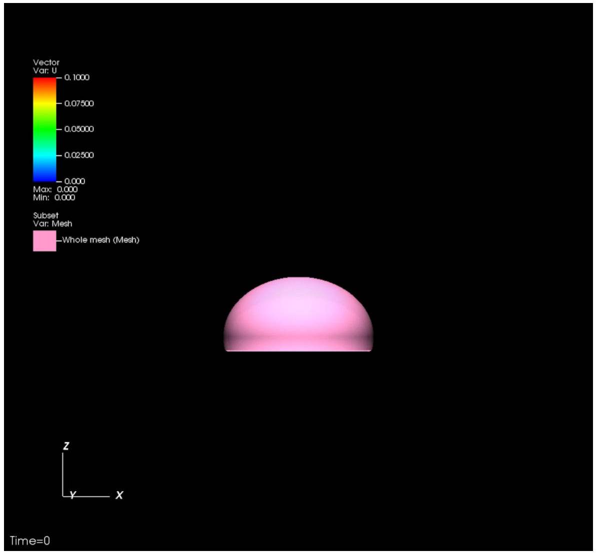
A) Tiny insects and odor tracking, B) numerical simulations of filter feeding, C) rhodamine dye leaching form the surface of a reef of cleaned skeletons showing dynamics of larval settlement.

Active behavior in fluid: a challenging problem

From the Fluid Dynamics perspective:

- Resolving the fluid velocity field around active swimmers is a **difficult and computationally expensive problem**!
- Consequently, most fluid-structure interaction work on active organism swimming considers only 1-3 organisms at a time, particularly in 3D.

This is accomplished by solving a fluid structure interaction problem.



3D Jellyfish Simulation
Laura Miller and Alex Hoover

Fluid-structure interaction problems

In Peskin's *immersed boundary method* the equations of motion for an elastic, incompressible structure are coupled with a viscous, incompressible fluid (Navier-Stokes equations) as follows:

$$\left.\begin{aligned}
&\rho\left[\frac{\partial \mathbf{u}}{\partial t}(\mathbf{x},t)+\mathbf{u}(\mathbf{x},t)\cdot\nabla\mathbf{u}_t(\mathbf{x},t)\right]=-\nabla p(\mathbf{x},t)+\mu\,\nabla^2\mathbf{u}(\mathbf{x},t)+\mathbf{f}(\mathbf{x},t)\\
&\nabla\cdot\mathbf{u}(\mathbf{x},t)=0
\end{aligned}\right\}\ \boxed{\text{Fluid Equations}}$$

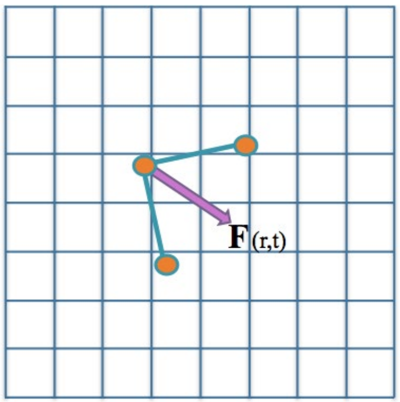
$$\left.\begin{aligned}
&\mathbf{f}(\mathbf{x},t)=\int \mathbf{F}(q,t)\,\delta(\mathbf{x}-\mathbf{X}(q,t))\,dq\\
&\frac{d\mathbf{X}(q,t)}{dt}=\mathbf{U}(\mathbf{X}(q,t))=\int \mathbf{u}(\mathbf{x},t)\,\delta(\mathbf{x}-\mathbf{X}(q,t))\,d\mathbf{x}
\end{aligned}\right\}\ \boxed{\text{Fluid-Structure Interaction Eqns.}}$$

- **x**=(x,y) : Cartesian coordinates
- q: Lagrangian (material) point position
- **X**(q,t) : Physical position of material pt. *q*, at time *t*
- **u**(**x**,t): Eulerian velocity field
- **F**(q,t): Lag. Elastic force density due to deformations of the structure

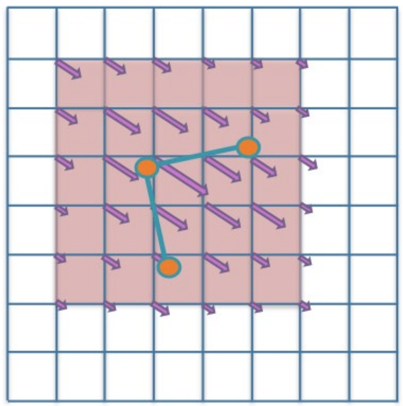
IB2d

Battista, WCS, Miller (2017) *Bioinspiration & Biomimetics*
Battista, WCS, Barrett, Miller (2018) *Mathematical Methods in the Applied Sciences*

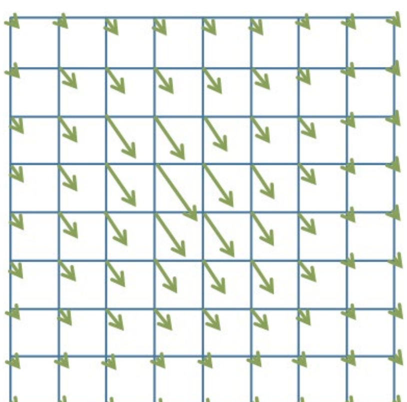
Step 1: Compute Elastic Force Density on *Immersed Body*



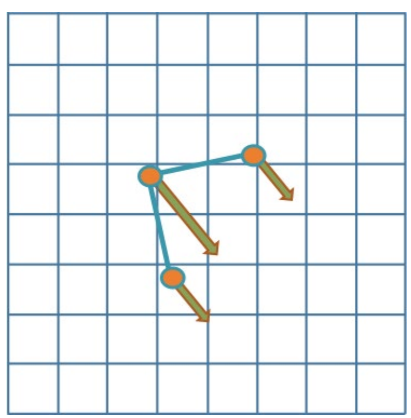
Step 2: Spread the elastic force from deformed body onto fluid



Step 3: Update the *fluid's* velocity



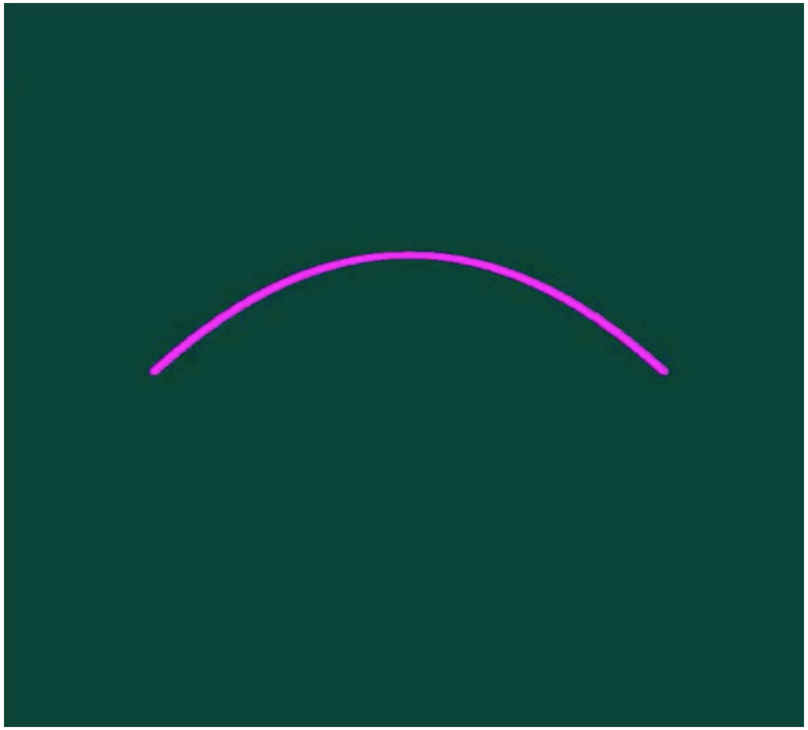
Step 4: Update the *immersed body's* position



Example:

Flexible Beam

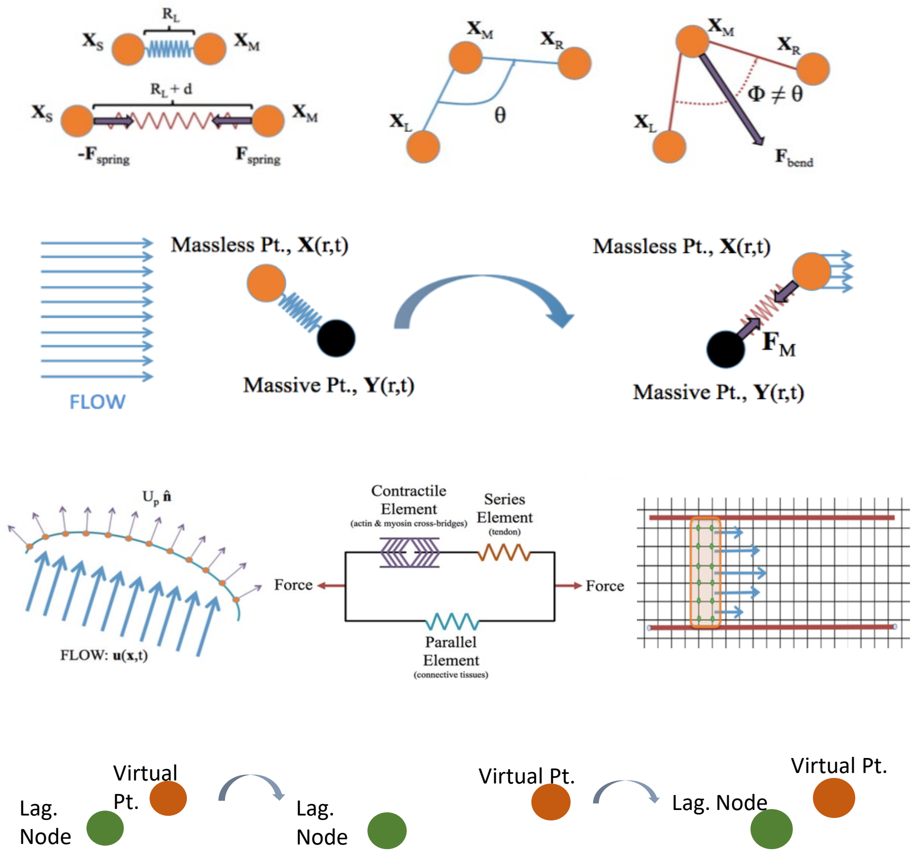
(movie)



IB2d

Battista, WCS, Miller (2017) *Bioinspiration & Biomimetics*
Battista, WCS, Barrett, Miller (2018) *Mathematical Methods in the Applied Sciences*

Built-in examples & contemporary material property models



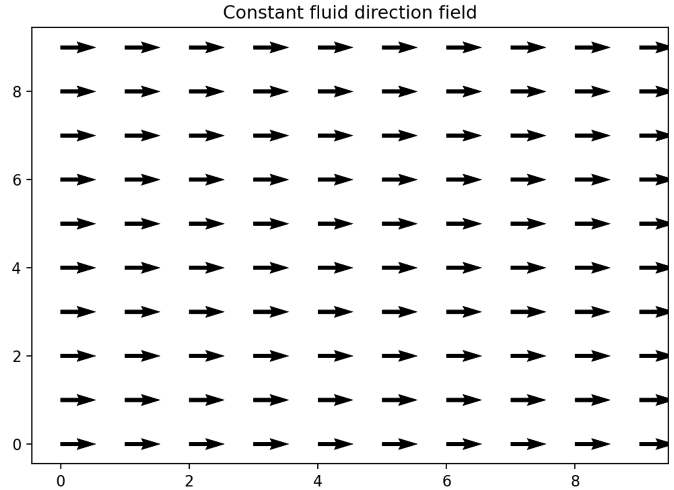
- Springs (Hookean, non-Hookean, damped)
- Beams
- Torsional Springs
- Target Points
- Porosity
- Poroelasticity
- Mass (w/ or w/o gravity)
- Electromagnetic-type contact models
- Muscle-Fluid-Structure Models
  - Force-Velocity / Length-Tension Model
  - 3-Element Hill Model

<u>NOTE</u>: 3D simulations can be especially challenging and are beyond the scope of IB2d. Packages include IBAMR (Boyce Griffith), COMSOL and Ansys Fluent.

Active behavior in fluid: a challenging problem

From the Collective Behavior perspective:

- Almost all individual-based models of collective behavior neglect fluid flow altogether.
- When this isn't the case, various sweeping assumptions are used:
  - The fluid is spatially and/or temporally constant
  - *Very* rough approximations are used for how the fluid might behave near large structures of importance, ignoring a lot of fluid physics.
  - Vortices and other such features are not resolved and largely ignored.



Modeling active behavior in dynamic flows

Our project is aimed at studying:

- The collective behavior of small organisms
- Whose effect on the fluid is **negligible**
- As they interact with larger organisms that **do** affect the fluid.

Applications target the mesoscale (~1 m).

Note: Small organism movement can often be formulated as vectorized systems of ODE and SDE, but this class of non-homogenous dynamical systems is largely *unstudied*.

This represents an interesting middle ground between CFD on the one hand, and population dynamics on the other!

Planktos: a modeling framework for active organismal behavior in dynamic flows

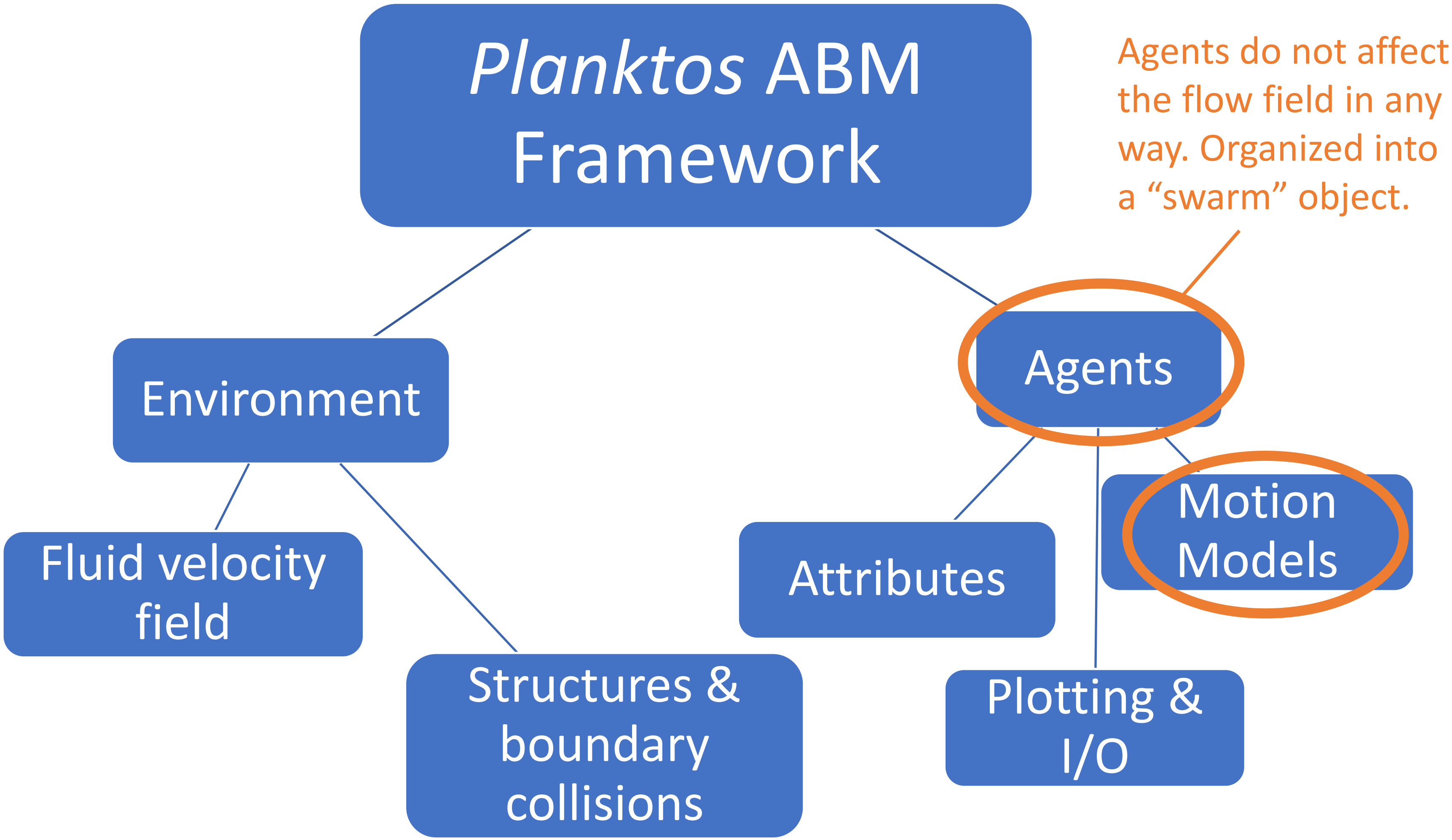
Planktos is a numerical simulation environment for agent-based and dynamical systems modeling that handles the specific challenges of *temporally and spatially heterogenous fluid-structure interaction data*.

- Aimed at (Monte Carlo) simulations in both 2D and 3D.
- This is **NOT** an FSI solver. Modeled organisms are assumed *small enough that their effect on the background flow is negligible*.
- Therefore, the fluid velocity field is constructed ahead of time (e.g. in IB2d, COMSOL, OpenFOAM, IBAMR, etc.)
- It is robust to generalized, user-defined organismal behavior!
- Written in Python (NumPy)
- Simulation visualization is included
- Online documentation available: *https://planktos.readthedocs.io/*

WCS, Battista, Hamlet, Miller (2022). *Bulletin Math Biol*. 84(72)

Planktos agent-based modeling framework

https://github.com/mountaindust/Planktos



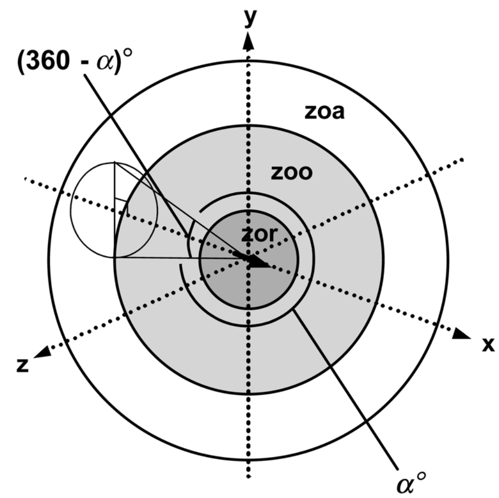
WCS, Battista, Hamlet, Miller (2022). *Bulletin Math Biol*. 84(72)

Modelling motion/behavior

- A python script can be used to specify general, coupled agent behavior including changes of state.
- Systems of ODE and SDE can be solved.
- Boundary conditions on any immersed structures and the environmental boundary must be specified.

Example: Three-zone model

(repulsion, alignment, attraction)



(Couzin *et al.* 2002, *J Theor Biol* 218)

As far as we are aware, these type of models have not been studied in fluid flow around immersed structures!

Modelling motion/behavior

Stochastic differential equations for a Wiener processes:

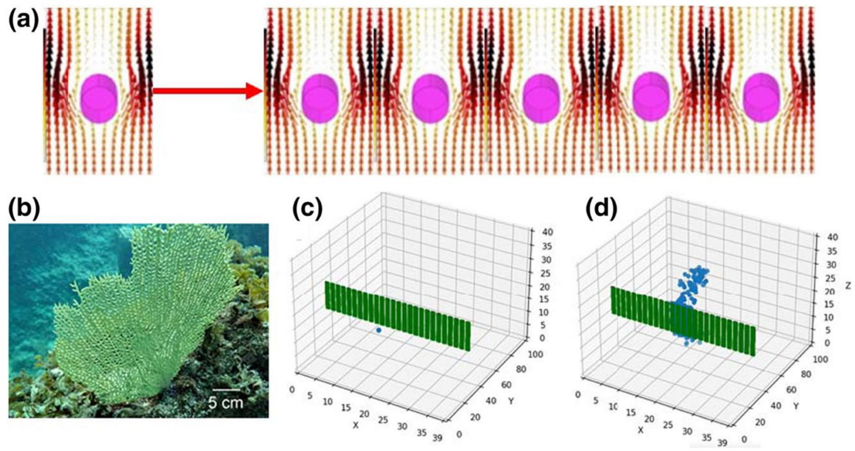
$$d\mathbf{X_t} = \underbrace{\boldsymbol{\mu}(\mathbf{X_t}, t)}_{\substack{\text{deterministic}\\ \text{drift}}}\ dt + \underbrace{\sigma(\mathbf{X_t}, t)}_{\text{diffusion coeff.}}\ d\mathbf{W_t}$$

with

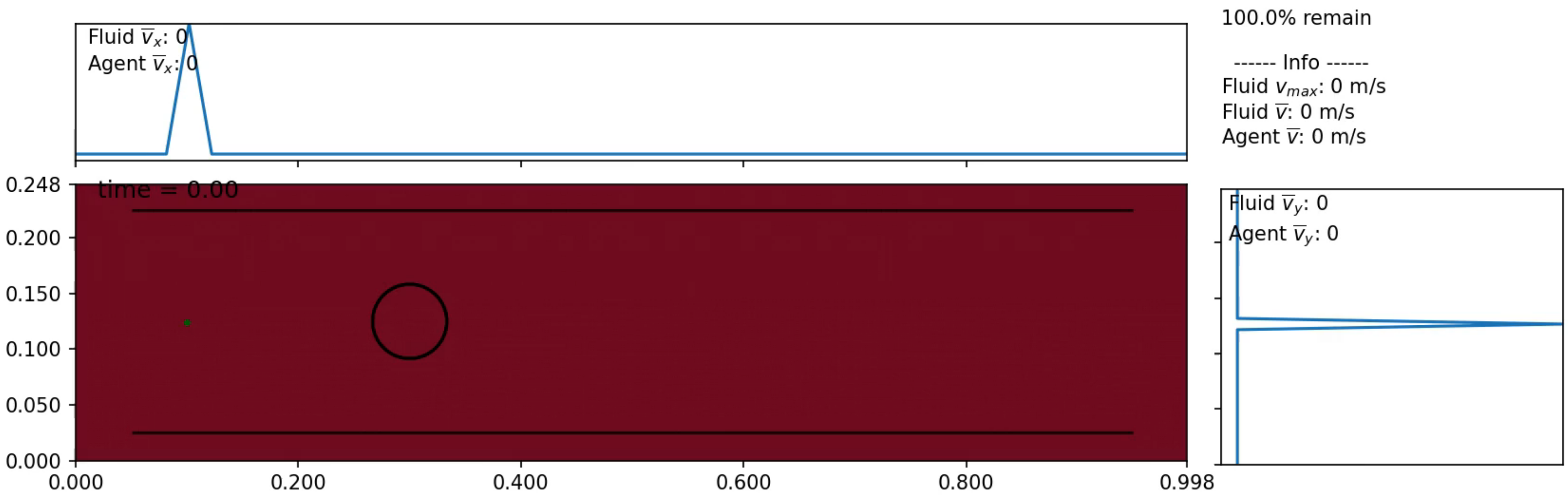
$$\boldsymbol{\mu}(\mathbf{X_t}, t) = \underbrace{\mathbf{u}(\mathbf{X_t}, t)}_{\text{fluid drift}} + \underbrace{\mathbf{f}(\mathbf{X_t}, t)}_{\substack{\text{agent}\\ \text{movement}}}$$

Currently, these are assumed to be uncoupled and $\sigma(t)$ is assumed to be spatially constant. Solved with Euler-Maruyama method (strong order-1).

This can be used for different Brownian models – for instance, a null model for plankton capture by immersed structures.

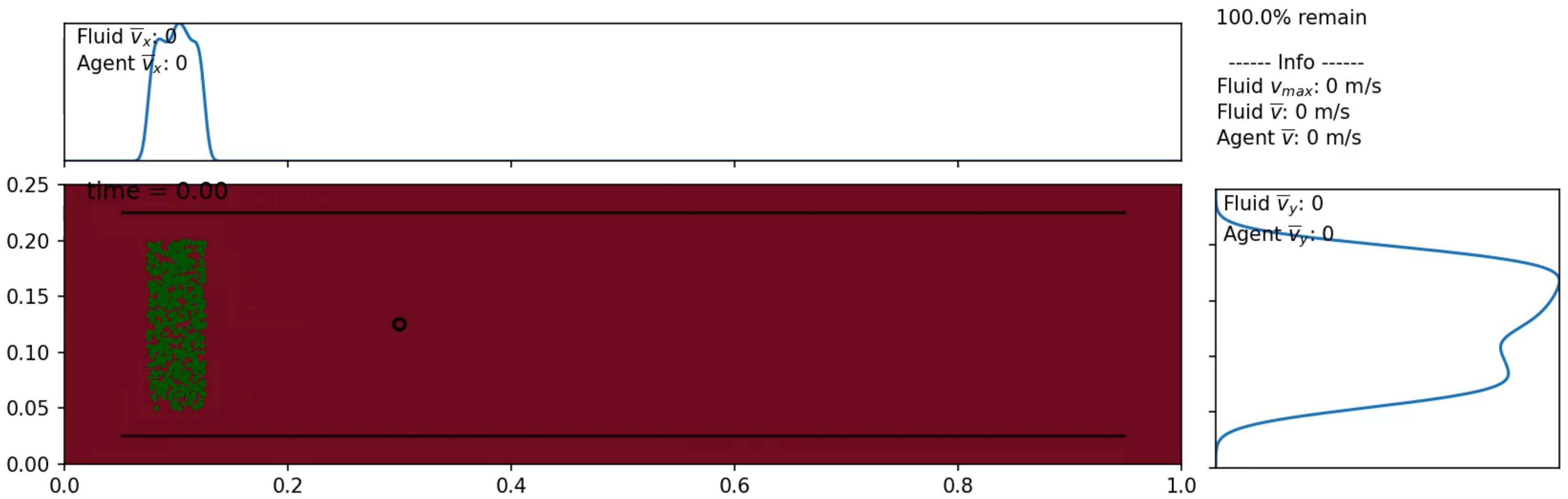


2D example of Brownian simulation in Planktos



- Flow generated in IB2d: unsteady channel flow around an immersed cylinder w/ periodic boundary conditions
- Agents can exit the domain (homogeneous Dirichlet BC)
- Agents experience inelastic collisions with immersed boundaries (frictionless, mass of particles assumed to be zero).
- Fluid vorticity is plotted; side plots are Gaussian kernel density estimates for agent positions

2D example of Vicsek model simulation in Planktos

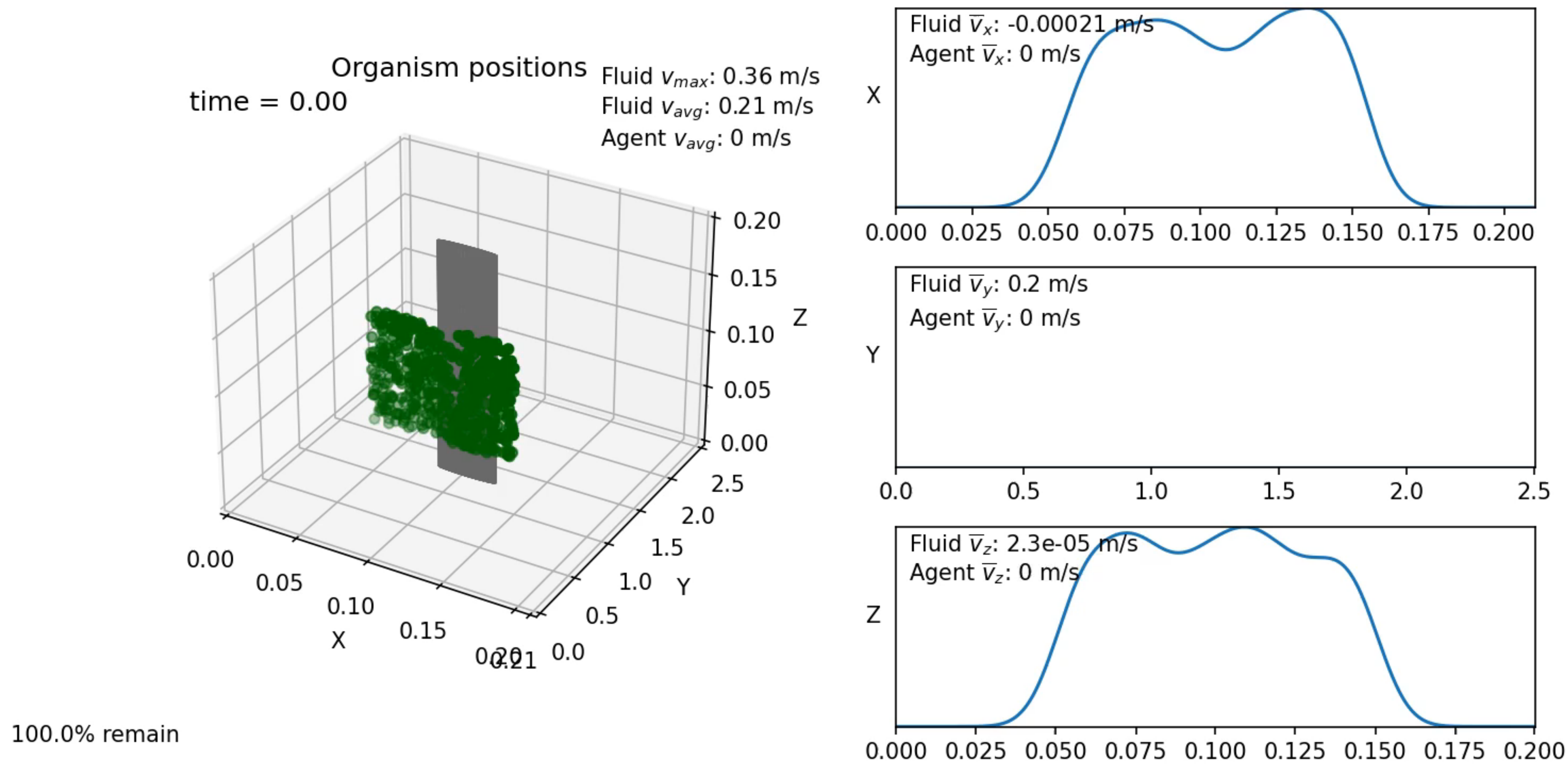


<u>Other options include</u>:

- Agents can stick to immersed structures on contact – e.g. for a model of particle capture
- Fluid domain can be tiled (assuming periodic fluid BC)
- Data can be exported to csv, json, or vtk for external analysis and visualization

Tutorial-style examples are included to get started!

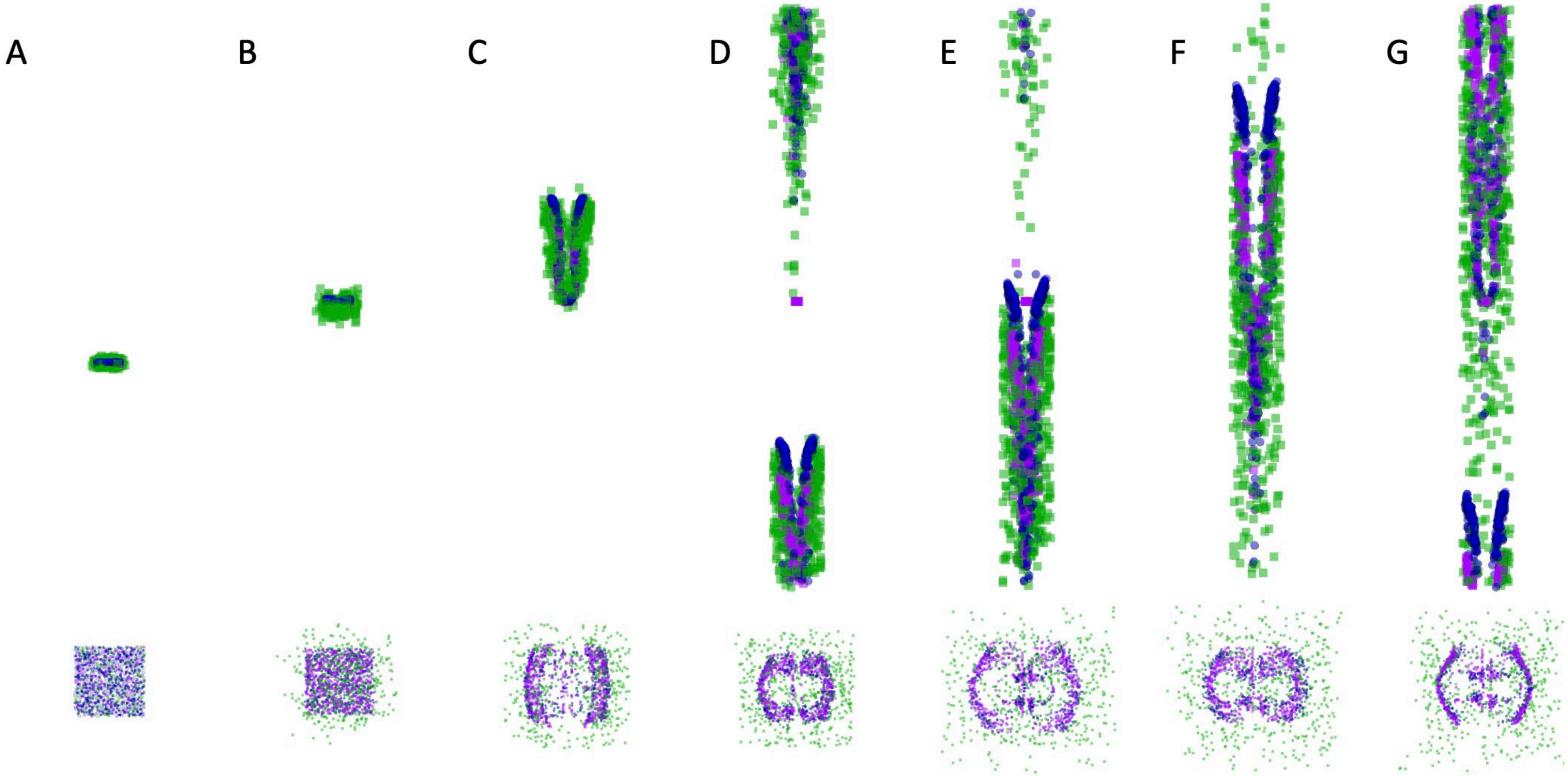
3D Vicsek model around immersed cylinder in flow



3D visualization is hard!

- Matplotlib will only display cubic aspect ratios, agents sometimes get lost near immersed mesh/STL.
- Current work: leverage VTK libraries for improved visualization.

Collective motion comparison: passive, vs. Vicsek, vs. Brownian around a 3D cylinder (not shown)

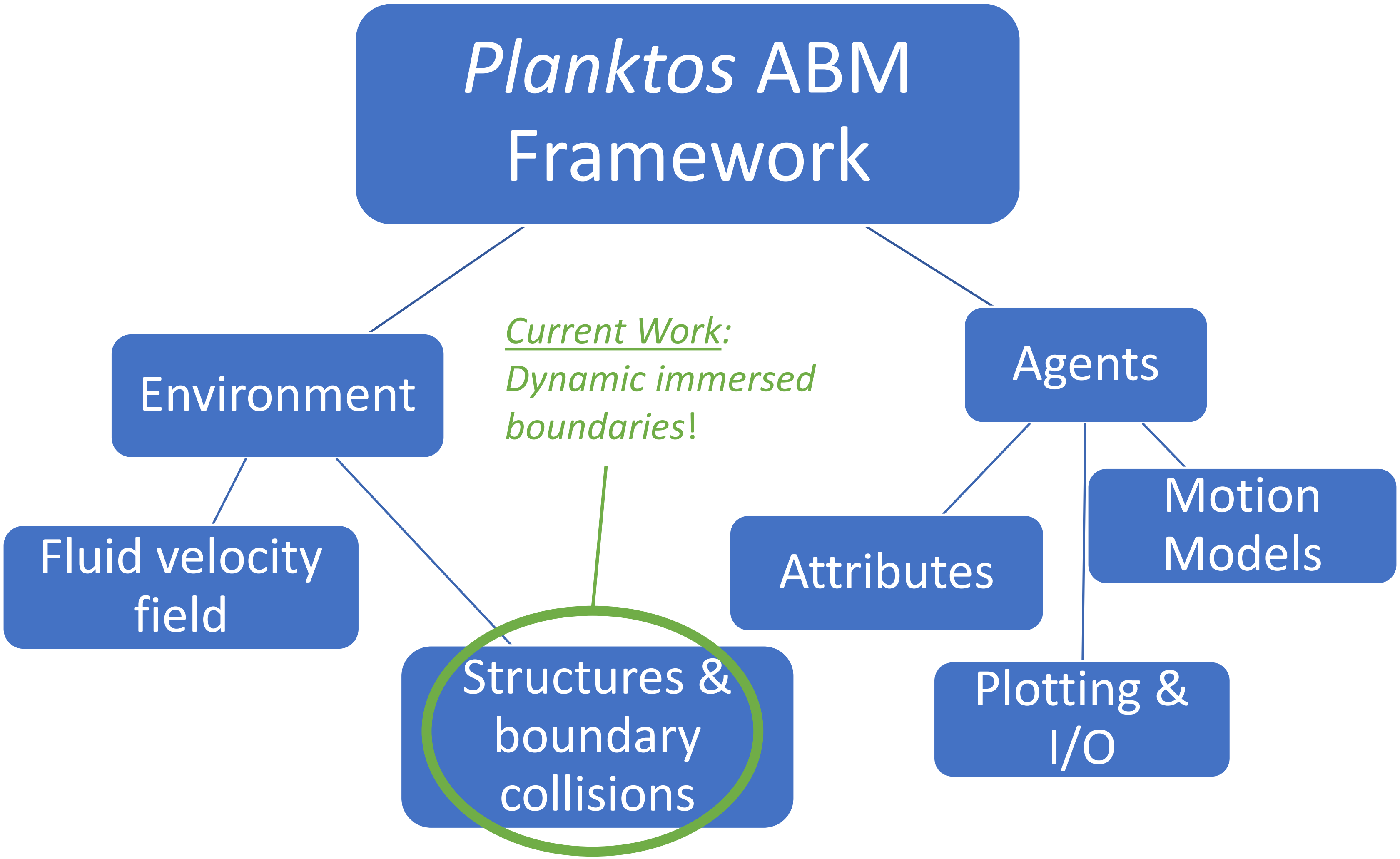


A-G: 0, 1.25, 2.5, 5.0, 7.5, 10, and 12.5 seconds, visualized in ParaView from *Planktos* VTK output.

WCS, Battista, Hamlet, Miller (2022). *Bulletin Math Biol*. 84(72)

Planktos agent-based modeling framework

https://github.com/mountaindust/Planktos



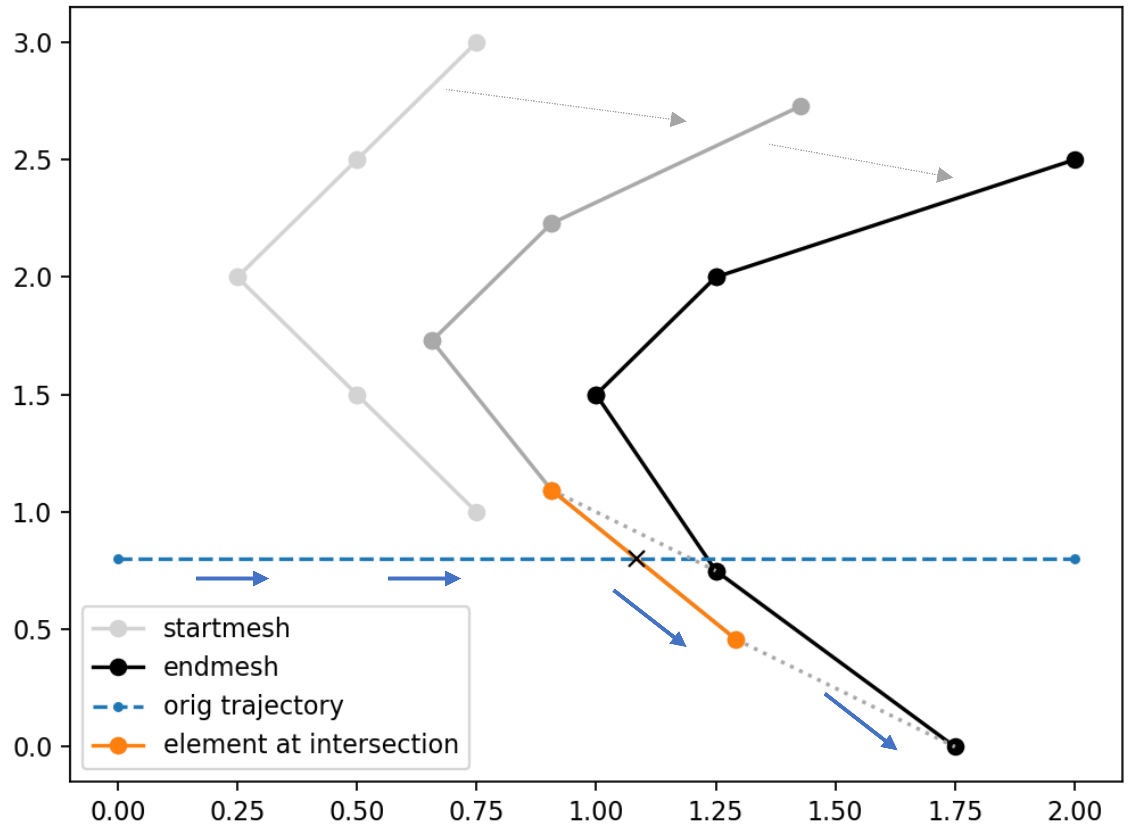
WCS, Battista, Hamlet, Miller (2022). *Bulletin Math Biol*. 84(72)

Latest work in *Planktos*: moving immersed boundaries

Note: even though this is not an FSI problem, there are major challenges.

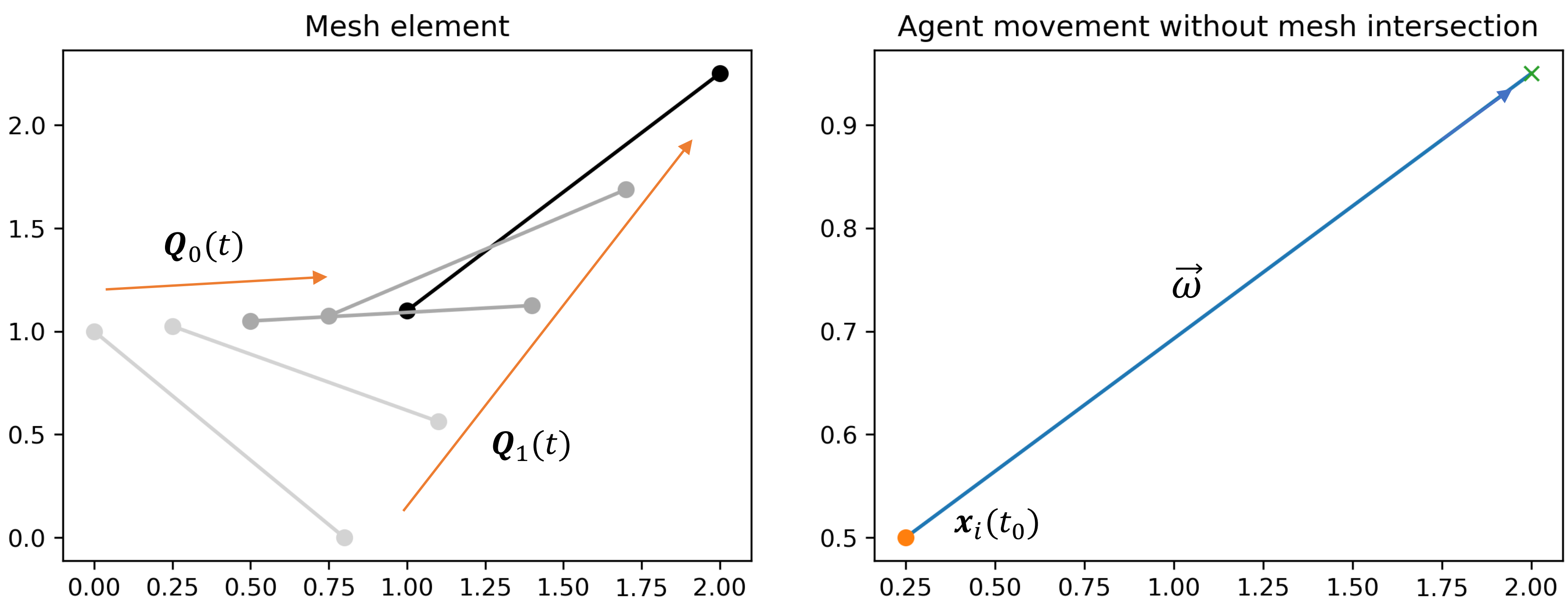
~1000s of individual agents interact with ~1000s of mesh elements that must be interpolated in both time and space. Numerical efficiency is important!

2D Example:



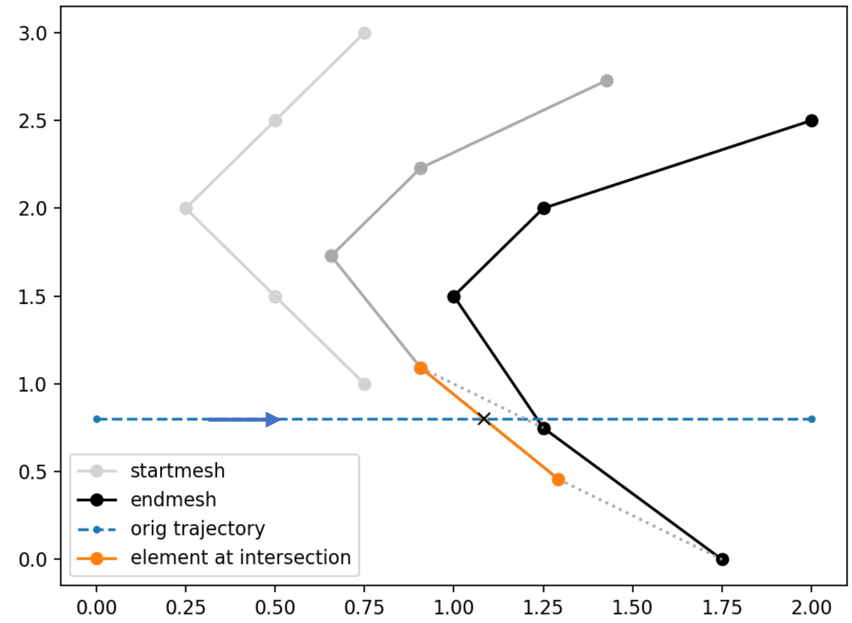
Mathematics of boundary interactions in *Planktos*

1. For each agent in a given timestep, identify any intersections with immersed boundary elements (line segments).
   a) <u>To start</u>: coarse subsetting of the mesh using length of travel and greatest distance of mesh vertex movement during timestep Δt.
   b) In space + time, each mesh element is a multilinear polynomial from $(t_0, t_0 + \Delta t)$. On the same interval, each agent's movement is given by linear interpolation $\boldsymbol{x}_i(t) = \boldsymbol{x}_i(t_0) + \vec{\omega}\tau\Delta t$ with $\tau \in [0,1]$.



Mathematics of boundary interactions in *Planktos*

1. For each agent in a given timestep, identify any intersections with immersed boundary elements (line segments).
   c) <u>Then</u>: we substitute the agent movement equation into the multilinear polynomial to get a quadratic equation.
      i. If roots in τ lie within $[0,1]$, then the agent intersects the interpolated (infinite) line specified by the mesh element.
      ii. If the intersection is also between the interpolated vertices for the mesh element, then a boundary interaction occurs.



Do this for all agents.

Mathematics of boundary interactions in *Planktos*

2. Assume inelastic collisions between agents and mesh elements where the mesh is a frictionless surface of infinite mass compared to the agent. Agent momentum is neglected.
   a) Agent velocity while in contact with a mesh element $\boldsymbol{Q}$ can be broken into two components: (1) velocity parallel to the surface (from the agent's movement prior to collision) and (2) velocity perpendicular to the surface (from mesh element movement).

$$\frac{d\mathbf{x}_i}{dt} = \frac{d\mathbf{x}_{agent\|\mathbf{Q}}}{dt} + \frac{d\mathbf{x}_{elem\perp\mathbf{Q}}}{dt}$$

   b) Velocity parallel to the surface is given via projection of the agent's original Euler-step movement $\vec{\mathbf{v}}$ onto $\boldsymbol{Q}$:

$$\frac{d\mathbf{x}_{agent\|\mathbf{Q}}}{dt} = \frac{\vec{\mathbf{Q}}(t)(\vec{\mathbf{Q}}(t)\cdot\vec{\mathbf{v}})}{||\vec{\mathbf{Q}}(t)||^2}$$

Mathematics of boundary interactions in *Planktos*

2. Assume inelastic collisions between agents and mesh elements where the mesh is a frictionless surface of infinite mass compared to the agent. Agent momentum is neglected.

   The location of the agent on the mesh element can be given in barycentric coordinates as

$$\mathbf{x}(t) = \mathbf{Q}_0(t) + s(t)\vec{\mathbf{Q}}(t) \quad \longrightarrow \quad s(t) = \frac{||\mathbf{x}(t) - \mathbf{Q}_0(t)||}{||\mathbf{Q}(t)||}$$

   c) Velocity orthogonal to the surface can then be found by taking the derivative of this equation and projecting onto a vector orthogonal to $\boldsymbol{Q}$.

$$\frac{d\mathbf{x}_{elem}}{dt} = \frac{d\mathbf{Q}_0}{dt} + s(t)\frac{d\mathbf{Q}}{dt} + \frac{ds}{dt}\mathbf{Q}(t)$$

$$\frac{d\mathbf{x}_{elem\perp\mathbf{Q}}}{dt} = \frac{\mathbf{Q}_\perp(t)\left[\mathbf{Q}_\perp(t)\cdot\left(\frac{d\mathbf{Q}_0}{dt} + \frac{d\mathbf{Q}}{dt}\frac{||\mathbf{x}(t)-\mathbf{Q}_0(t)||}{||\mathbf{Q}(t)||}\right)\right]}{||\mathbf{Q}_\perp(t)||^2}$$

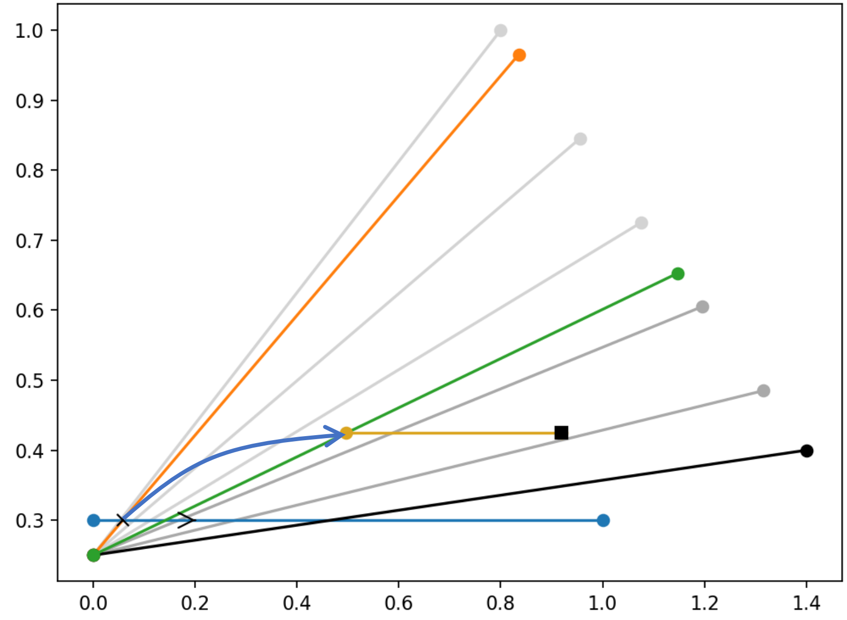
Mathematics of boundary interactions in *Planktos*

3. The resulting ODE is equivalent to a non-autonomous linear system with continuous coefficients – a unique solution always exists, and we can solve for it numerically.

4. An agent can leave the mesh element in two ways:

   a) Mesh element rotation can result in separation when the velocity of the element exceeds that of the agent in the same direction.

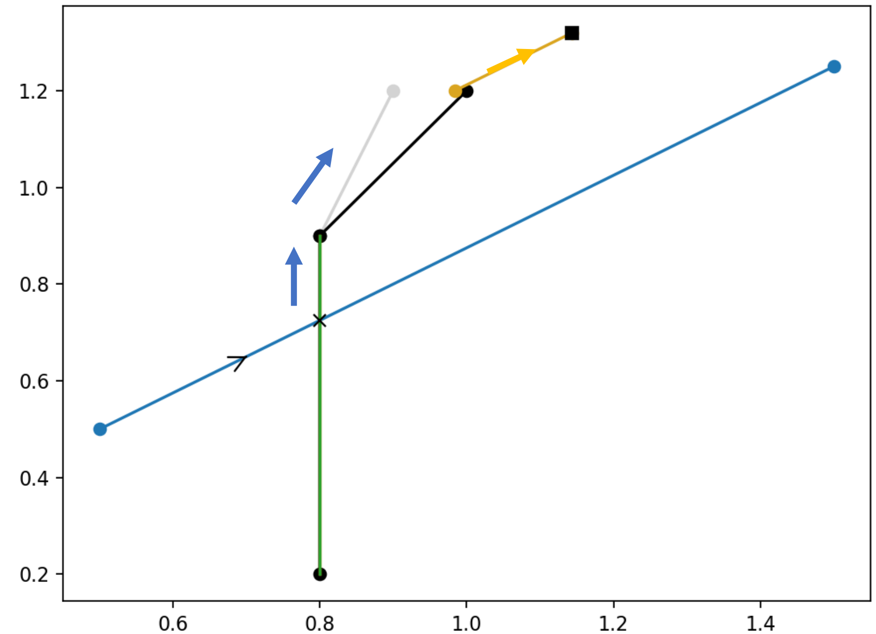
Algorithm: Detect any sign changes in the difference of the two velocities orthogonal to the element at $\boldsymbol{x}_i(t)$ and use a root finding algorithm to find the time of separation.



Mathematics of boundary interactions in *Planktos*

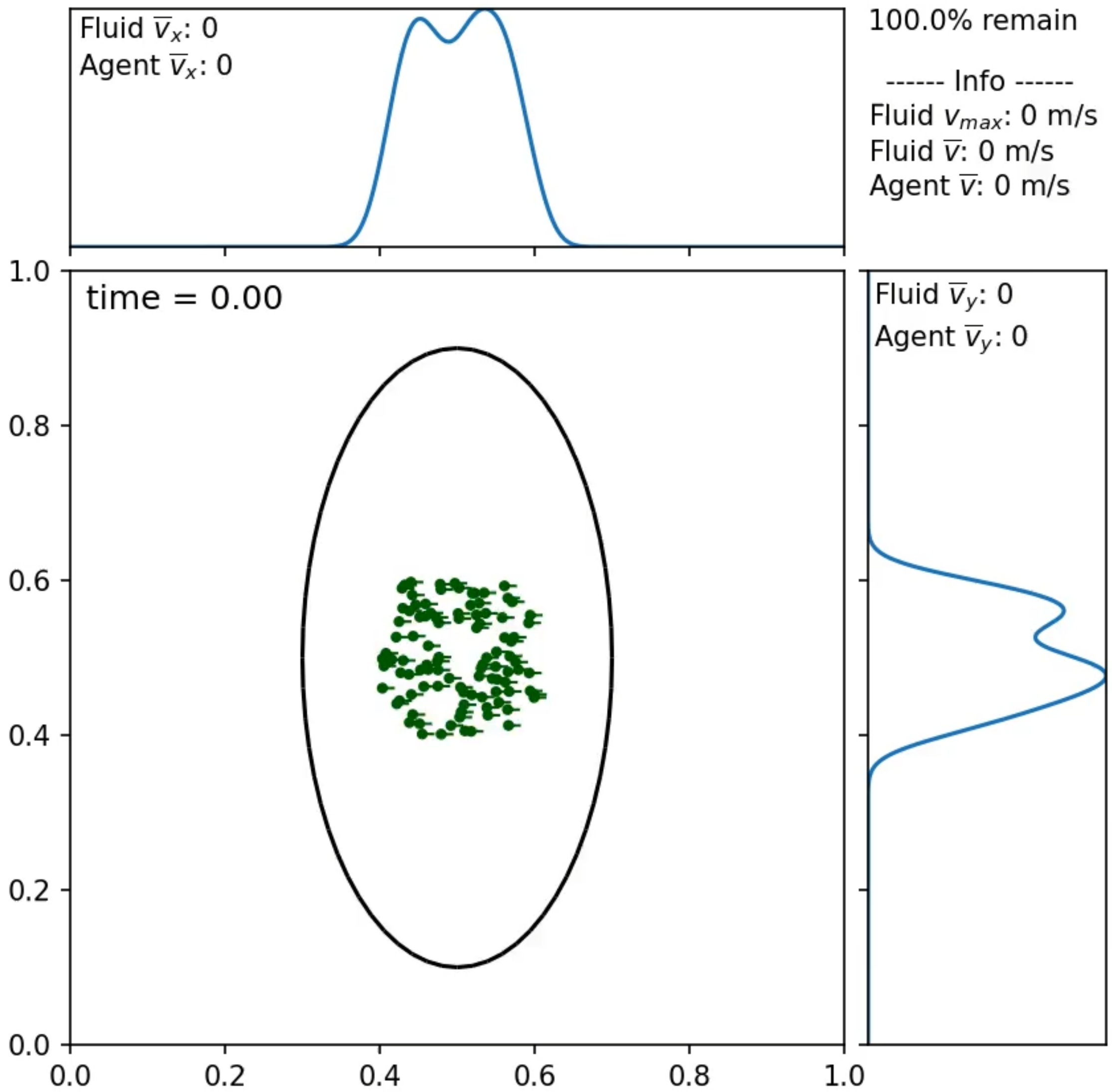
3. <u>An agent can leave the mesh element</u> in two ways:
   b) The agent can reach the edge of the mesh element.

Algorithm: Detect if the agent moves past one of the two endpoints, $\boldsymbol{Q}_0(t)$ or $\boldsymbol{Q}_1(t)$ (details suppressed). Then solve the nonlinear LSQ problem $||\boldsymbol{x}(t) - \boldsymbol{Q}_0(t)|| = 0$ for time t. Then continue movement along original trajectory.

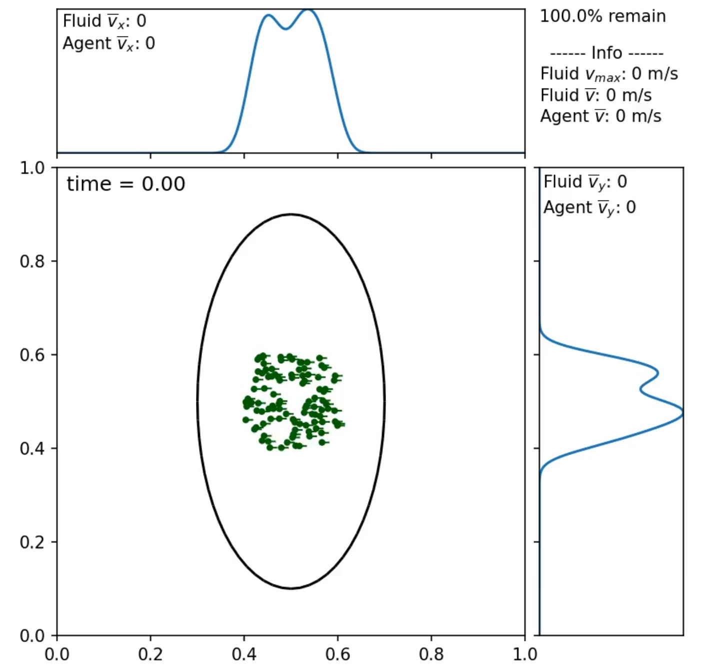


Recursion occurs for connected mesh elements or further collisions.

Test example: Brownian agents in poroelastic rubberband



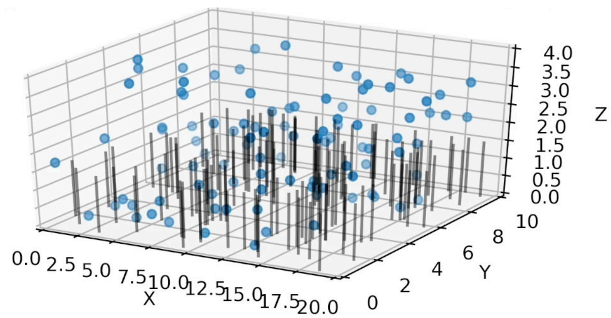
Future work in *Planktos*!



- Chemical gradient following behavior
- Comparison studies of collective behavior
- Dynamic loading of 3D fluid data
  - Temporal data can be huge
  - Interpolation makes it even worse
- 3D VTK visualization with 2D projection plots
- Moving immersed boundaries in 3D!

<u>Biological Questions</u>: How do small-scale flow patterns affect particle capture? What is the collective effect of coupled and reactive behaviors on small animal predation?

Thank you for your attention!



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More current work: small insect search strategies

An isolated parasitoid wasp must efficiently search a large area for small hosts.

An ***intermittent search strategy*** may be optimal.

Phase 1: A localized, Brownian search pattern in which the target can be detected.

Phase 2: Ballistic (straight-line) motion to a new location – target cannot be detected.

The survival probability $p_i(x,t)$ that, when the searcher starts at time $t=0$ in state i, the target has not yet been found by time t satisfies the *backward Kolmogorov equations*

$$D\frac{\partial^2 p_1}{\partial x^2} + \frac{1}{\tau_1}\left[p_2(x,t) - p_1(x,t)\right] = \frac{\partial p_1}{\partial t}$$
$$V\frac{\partial p_2}{\partial x} + \frac{1}{\tau_2}\left[p_1(x,t) - p_2(x,t)\right] = \frac{\partial p_2}{\partial t}$$

Bénichou *et al.* (2005). Optimal search strategies for hidden targets, *Phys Rev Letters*

More current work: small insect search strategies

The survival probability $p_i(x,t)$ that, when the searcher starts at time $t = 0$ in state i, the target has not yet been found by time t satisfies the *backward Kolmogorov equations*

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$$V\frac{\partial p_2}{\partial x} + \frac{1}{\tau_2}\left[p_1(x,t) - p_2(x,t)\right] = \frac{\partial p_2}{\partial t}$$

…But this has not been considered in the context of

- Energy expenditure
- Fluid contexts, incl. *targets* that advect in the fluid velocity field
- Optimal forging theory

This is work with graduate student *Ryan Campbell*