Computational Methods for Modeling Multiphase Flow and Fluid-Structure Interaction in Coastal and Hydraulic Engineering Applications

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Outline

- Introduction and Motivation
- Some recent work on CutFEM and IFEM
- The Proteus Tookit for Computational Methods and Simulation

Acknowledgements

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- RPI: Sahni, Shepherd, Zhang
- MIT: Patera
- Wisconsin: Negrut, Rakhsha

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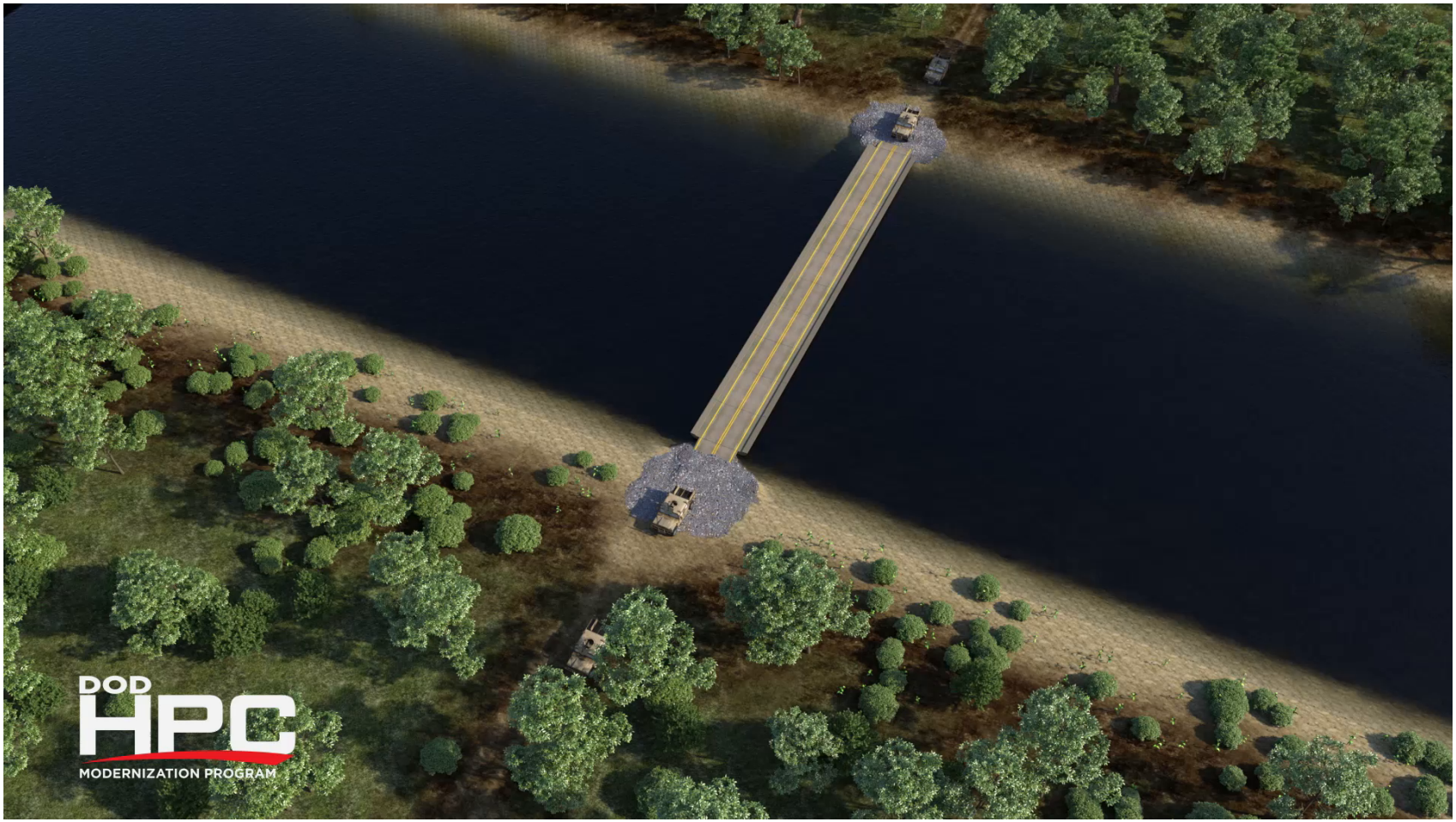
Improved Ribbon Bridge



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Wet Gap Crossing

- Provide assault and tactical bridge crossing capability
- Support loads up to MLC 80T/110W
- Helmand Example: 100 to 400 Meter Feet Wide, 8-18fps
- Is it stable?
- What are the loads on the overhead cable?

Beach Erosion and Deposition

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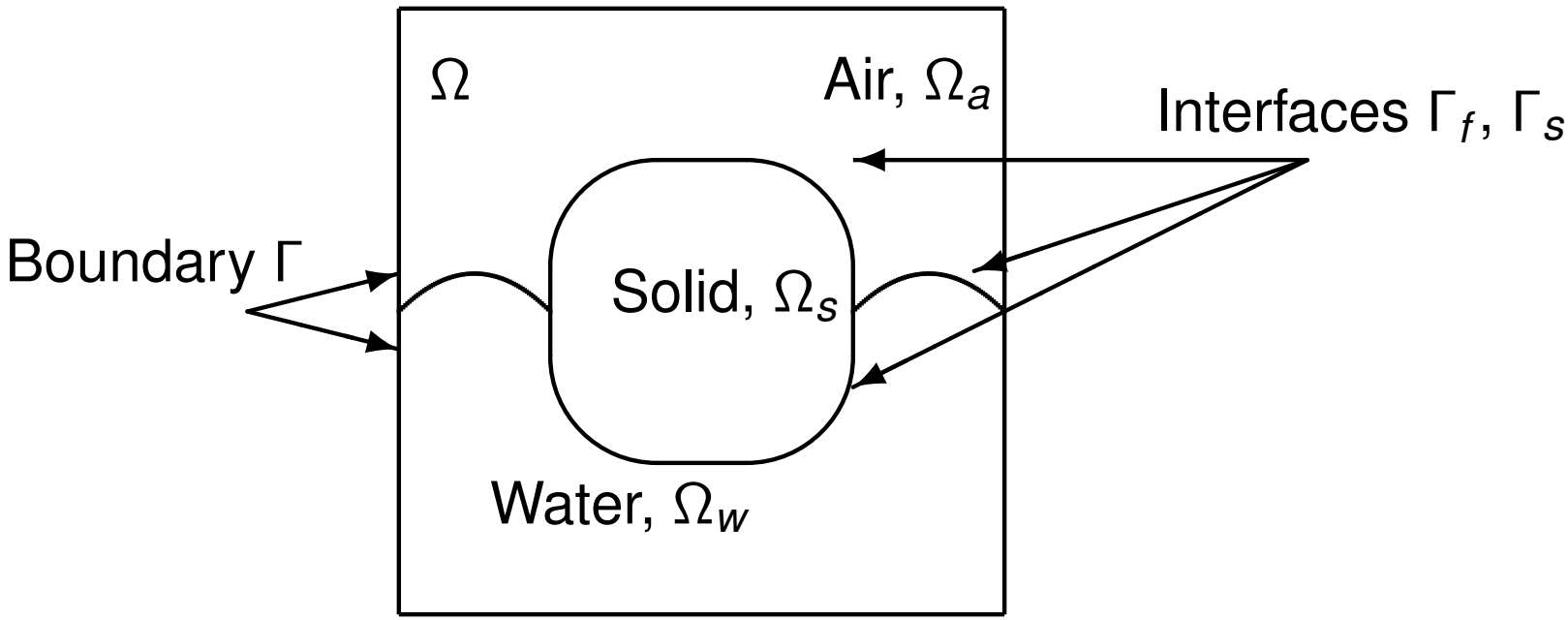
Simplified Domain



The fixed computational domain Ω and boundary Γ, with three dynamic subdomains Ω_w, Ω_a, and Ω_s and phase boundaries Γ_f and Γ_s

Numerical challenges and level set methods

- Dynamic interfaces: the fluid-fluid (air-water) interface, Γ_f, and the fluid-solid interface, Γ_s are moving in time.
- Changing topology: inter-granular contacts and bubble/droplet formation will occur, so the topology of $\Omega_s, \Omega_w, \Omega_a$ will change.
- In some important cases, ALE (conforming mesh deformation) is viable for the solid phase.
- Define "level set" functions ϕ_s and ϕ_f with the following properties:

$$\Omega_s(t) = \{\mathbf{x} \in \Omega | \phi_s(x,t) < 0\} \tag{1.1a}$$
$$\Omega_w(t) = \{\mathbf{x} \in \Omega | \phi_f(x,t) < 0\} \tag{1.1b}$$
$$\Omega_a(t) = \{\mathbf{x} \in \Omega | \phi_f(x,t) > 0\} \tag{1.1c}$$
$$\Gamma_s(t) = \{\mathbf{x} \in \Omega | \phi_s(x,t) = 0\} \tag{1.1d}$$
$$\Gamma_f(t) = \{\mathbf{x} \in \Omega | \phi_f(x,t) = 0\} \tag{1.1e}$$

Key ideas

- Represent the free boundary as an implicit surface, $\phi(\mathbf{x}, t) = 0$ (Osher and Sethian).
- Construct an equation for ϕ that is physically correct on the free boundary and reasonable in the rest of the domain:

$$\frac{\partial \phi}{\partial t} + \nabla \phi \cdot \mathbf{v} = 0 \tag{1.2}$$

- Used immersed boundary approximations to enforce boundary conditions along $\phi = 0$.
- Calculate the signed distance to $\phi = 0$:

$$\|\nabla \phi^d\| = 1 \tag{1.3}$$

- Do in a moving frame that allows the mesh to conform to a moving solid.

Two-Phase Flow, Part 1

1. Variable coefficient Navier-Stokes:

$$\begin{aligned} \nabla \cdot \mathbf{v}_+ &= 0 \\ \rho\left(\frac{\mathbf{v}_+ - \mathbf{v}_-}{\Delta t} + \mathbf{v}_+ \cdot \nabla \mathbf{v}_+\right) + \nabla \cdot [-2\mu\varepsilon(\mathbf{v}_+)] + \nabla p_+ &= \rho \mathbf{g} \end{aligned}$$

where

$$\rho = H_\epsilon(\phi_-)\rho_a + [1 - H_\epsilon(\phi_{-1})]\rho_w; \quad \mu = H_\epsilon(\phi_-)\mu_a + [1 - H_\epsilon(\phi_{-1})]\mu_w$$

2. Interface (level-set) transport:

$$\frac{\phi_+^* - \phi_-}{\Delta t} + \mathbf{v}_+ \cdot \nabla \phi_+^* = 0$$

Two-Phase Flow, Part 2

3. Fluid volume fraction advection

$$\frac{H_+^* - H_-}{\Delta t} + \nabla \cdot \left(H_+^* \mathbf{v}_+ \right) = 0$$

4. Redistance level set

$$\begin{aligned} \|\nabla \phi_+^{**}\| &= 1 \\ \phi_+^{**} &= 0 \text{ on } \phi_+^* = 0 \end{aligned}$$

5. Correct level set

$$\begin{aligned} H_\epsilon(\phi' + \phi_+^{**}) - H_+^* &= \epsilon_1 \Delta \phi' \\ \nabla \phi' \cdot \mathbf{n} &= 0 \text{ on } \partial\Omega \end{aligned}$$

$$\phi_+ = \phi' + \phi_+^{**} \quad H_+ = H_\epsilon(\phi' + \phi_+^{**})$$

See Quezada, Kuzmin, and K. 2019 for monolithic variant

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Three-Phase Level Set Formulation

$$\nabla \cdot \mathbf{v} = 0 \text{ in } \Omega \tag{1.4}$$

$$H_\epsilon(\phi_s)\left\{\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) + \nabla\cdot[-2\mu_f\varepsilon(\mathbf{v})] + \nabla p - \rho\mathbf{g}\right\} + \text{Nitsche}(\phi_s, \mathbf{v}) + [1 - H_\epsilon(\phi_s)](\mathbf{u} - \mathbf{u}_s) = 0 \text{ in } \Omega \tag{1.5}$$

Nitsche

- Integrate by parts on fluid momentum with no-slip only on Γ_s:

$$\int_{\Omega_f} [\mu \nabla \mathbf{v} \cdot \nabla \mathbf{w}] \, dV - \int_{\Gamma_s} \mu \nabla \mathbf{v} \cdot \mathbf{n} \mathbf{w} dS = 0$$

- Nitsche 71 showed how to enforce Dirichlet conditions consistently via penalty:

$$\int_{\Gamma_s} \left[-\mu(\phi) \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \mathbf{w} - \mu(\phi) \frac{\partial \mathbf{w}}{\partial \mathbf{n}} \mathbf{v} + C(h_e)(\mathbf{v} - \mathbf{v}_s)\mathbf{w} \right] dS$$

- We avoid explicitly meshing Γ_s by using the level set tools:

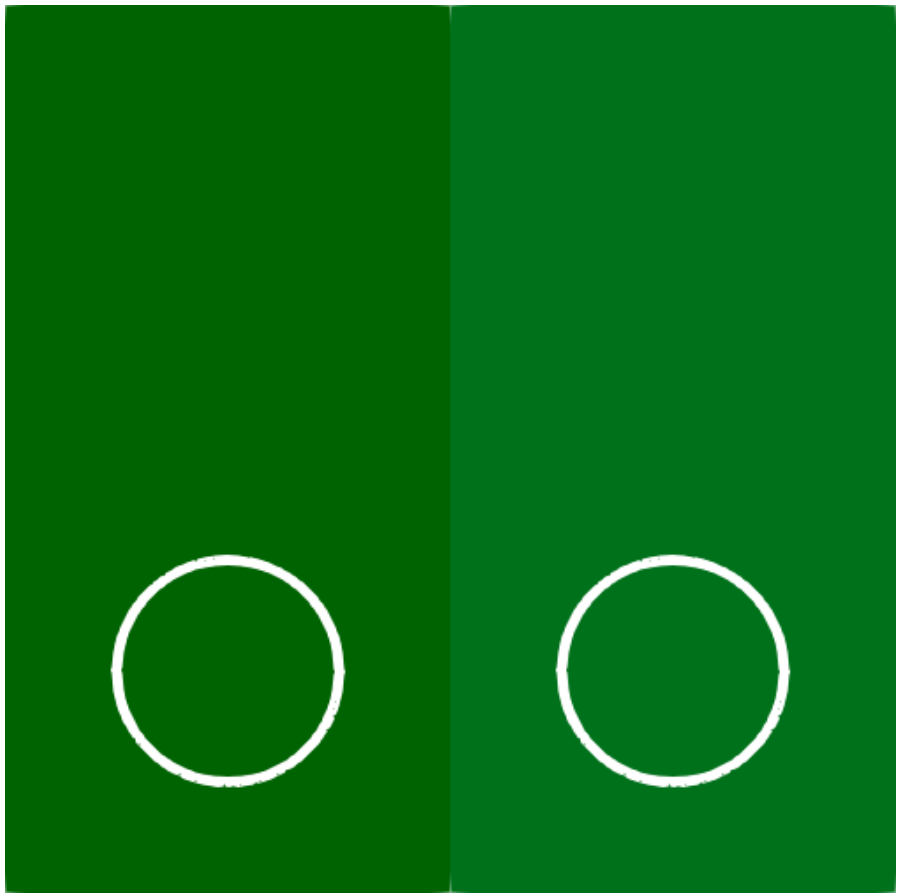
$$\int_{\Gamma_s} f dS = \int_{\Omega} \delta(\phi_s) f dV \approx \int_{\Omega} \delta_\epsilon(\phi_s) f dV$$

See [Osher and Fedkiw 2006]

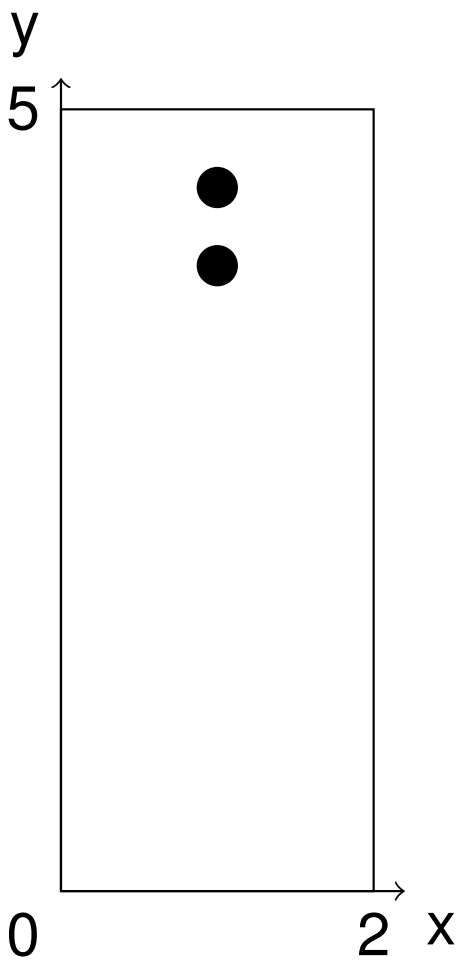
Prior Work in Proteus and Chrono

- We have developed a numerical laboratory combining Finite Element Methods (FEMs) from Proteus (https://proteustoolkit.org), and Discrete Element Methods (DEMs) from Chrono (https://projectchrono.org).
- The approach is based generally on level set methods, while using regularized Heaviside and Dirac functions to approximate volume and surface integrals on cells cut by the interface.
- These methods can produce qualitatively correct results for problems involving granular contacts and surface tension.

Surface Tension (Laplace-Beltrami Operator)



Sedimentation of two particles in a 2D channel



$$D = 0.25cm$$

$$\Omega = [0, 2] \times [0, 6]$$

$$c_1 = [1, 5]$$

$$c_2 = [1, 4.5]$$

$$\rho_s = 1.5$$

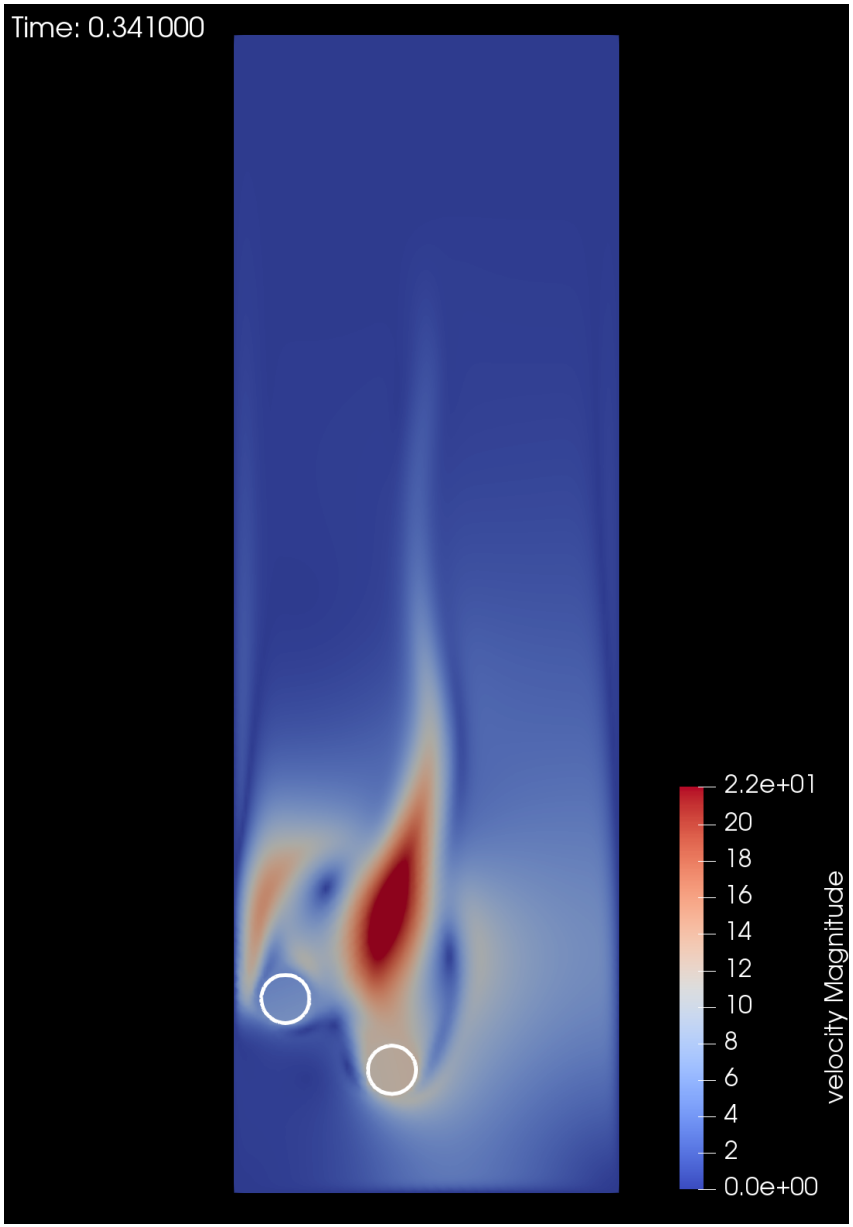
$$\rho_f = 1.0$$

$$\nu_f = 0.01$$

$$g = [0, -981, 0]$$

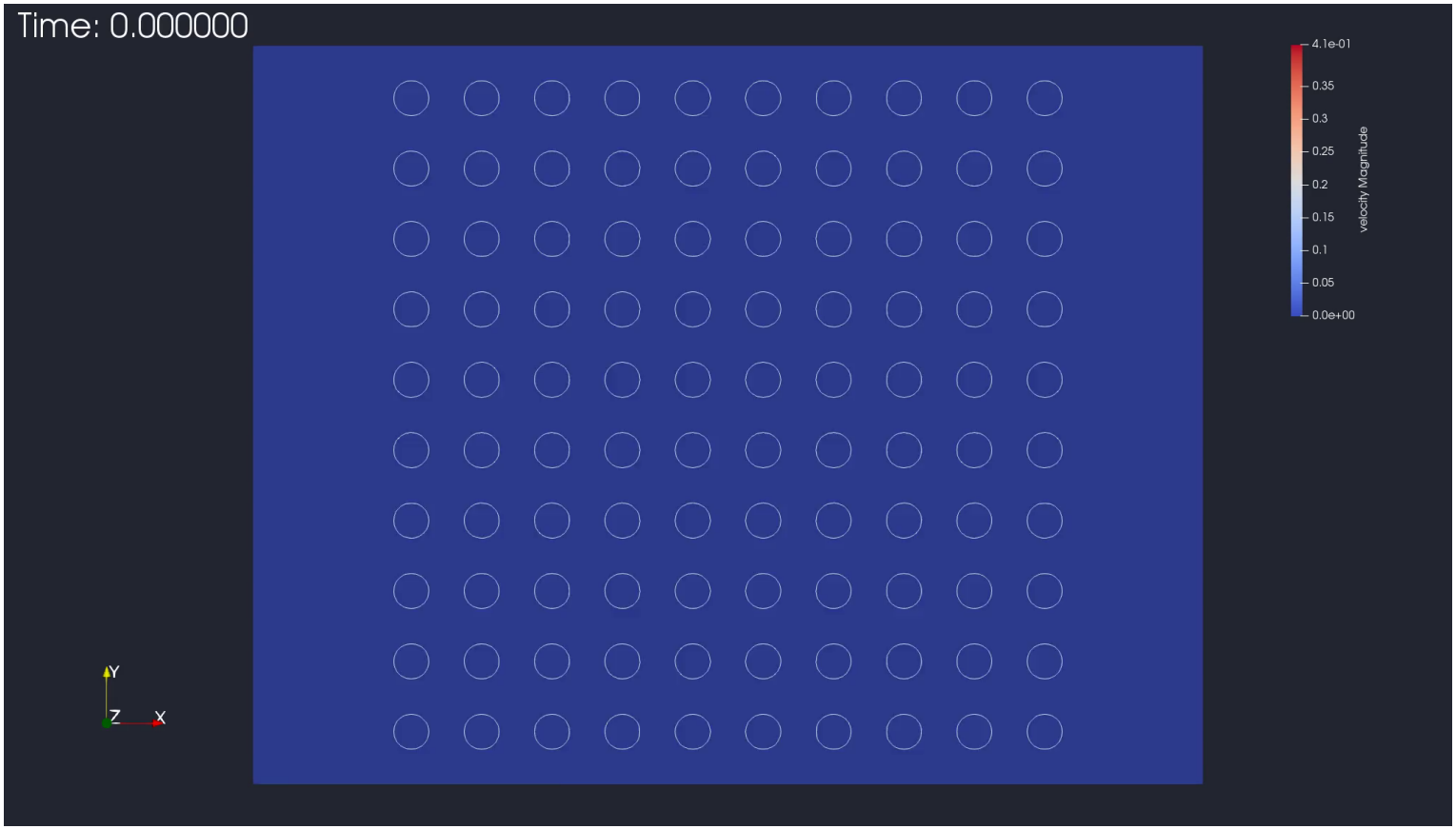
BC: no-slip + open top

Result

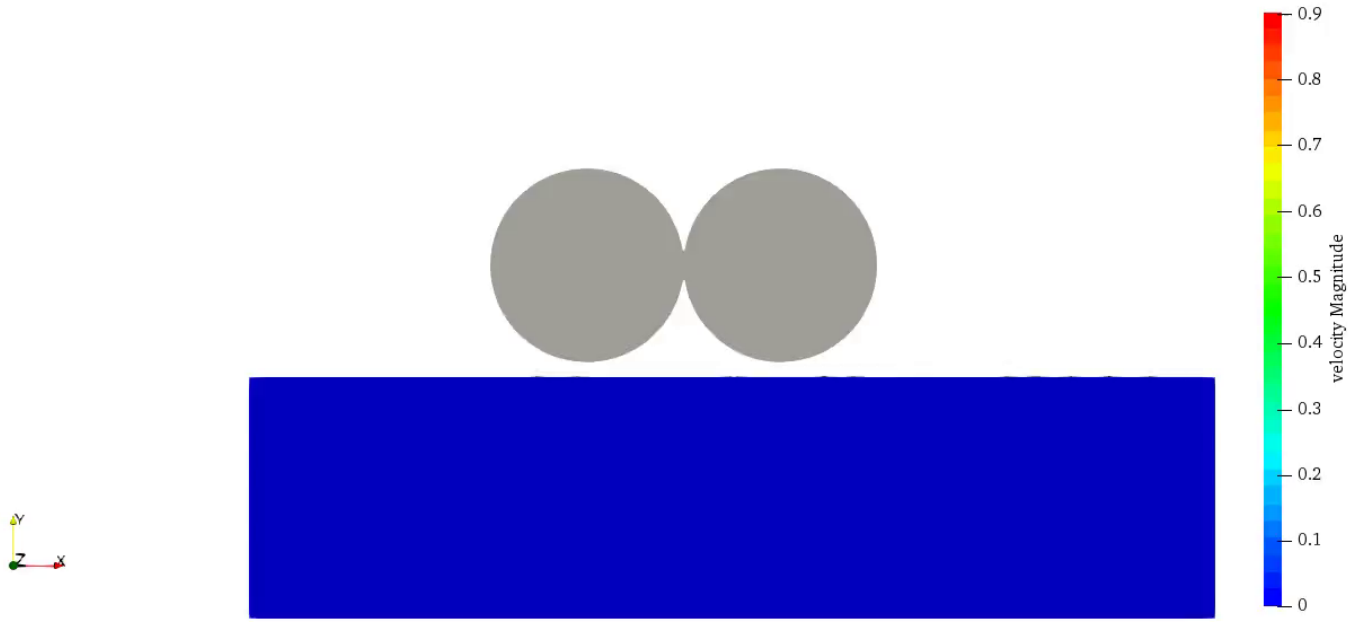


- $h = 1/32$, structured
- $\Delta t = 0.0005$
- $\mathbb{P}_2 - \mathbb{P}_1$

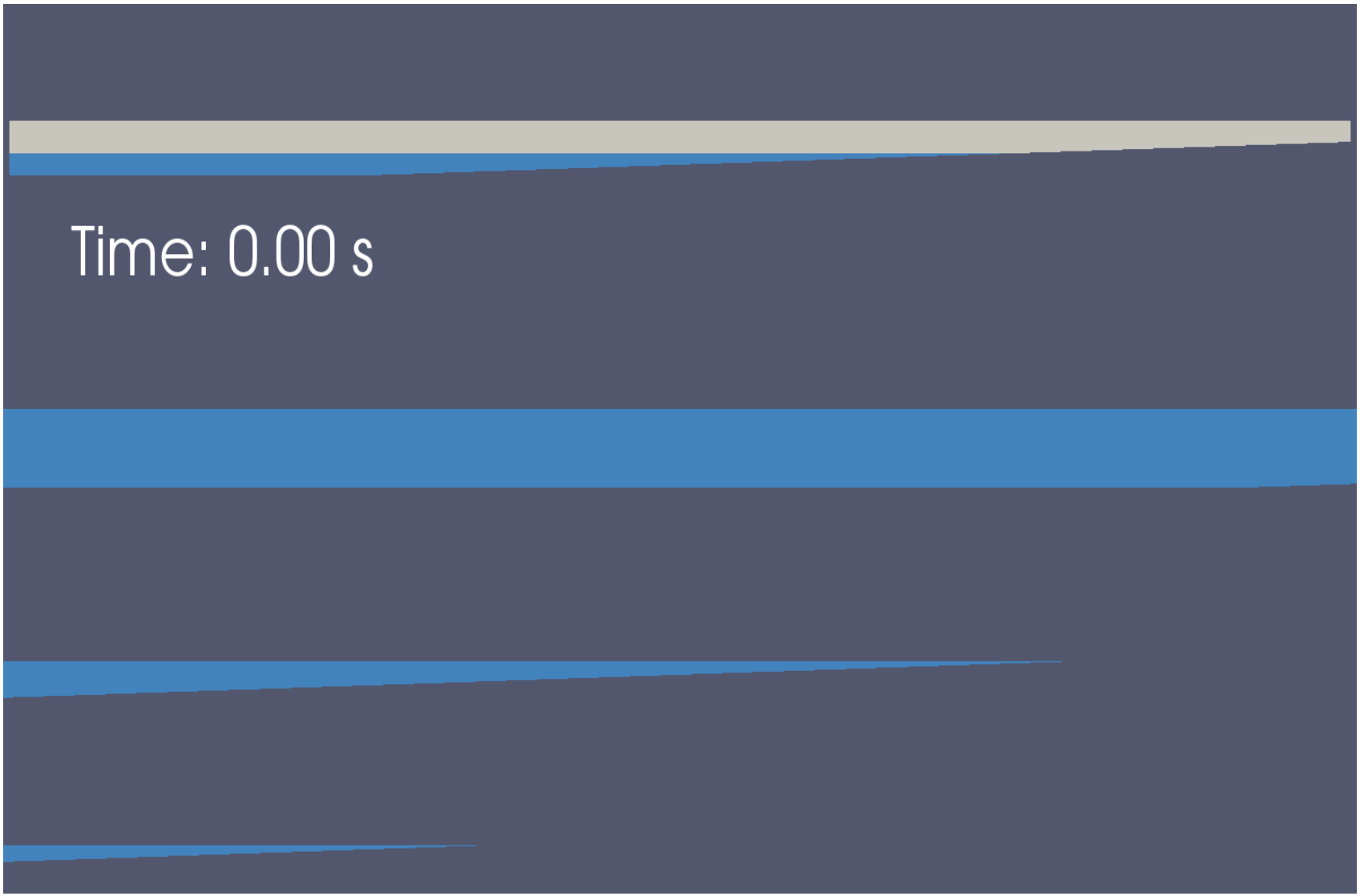
Settling


Time: 0.000000
4.1e-01
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0.0e+00
velocity Magnitude
Y
Z
X

Falling Spheres



Ting and Kirby Experiment



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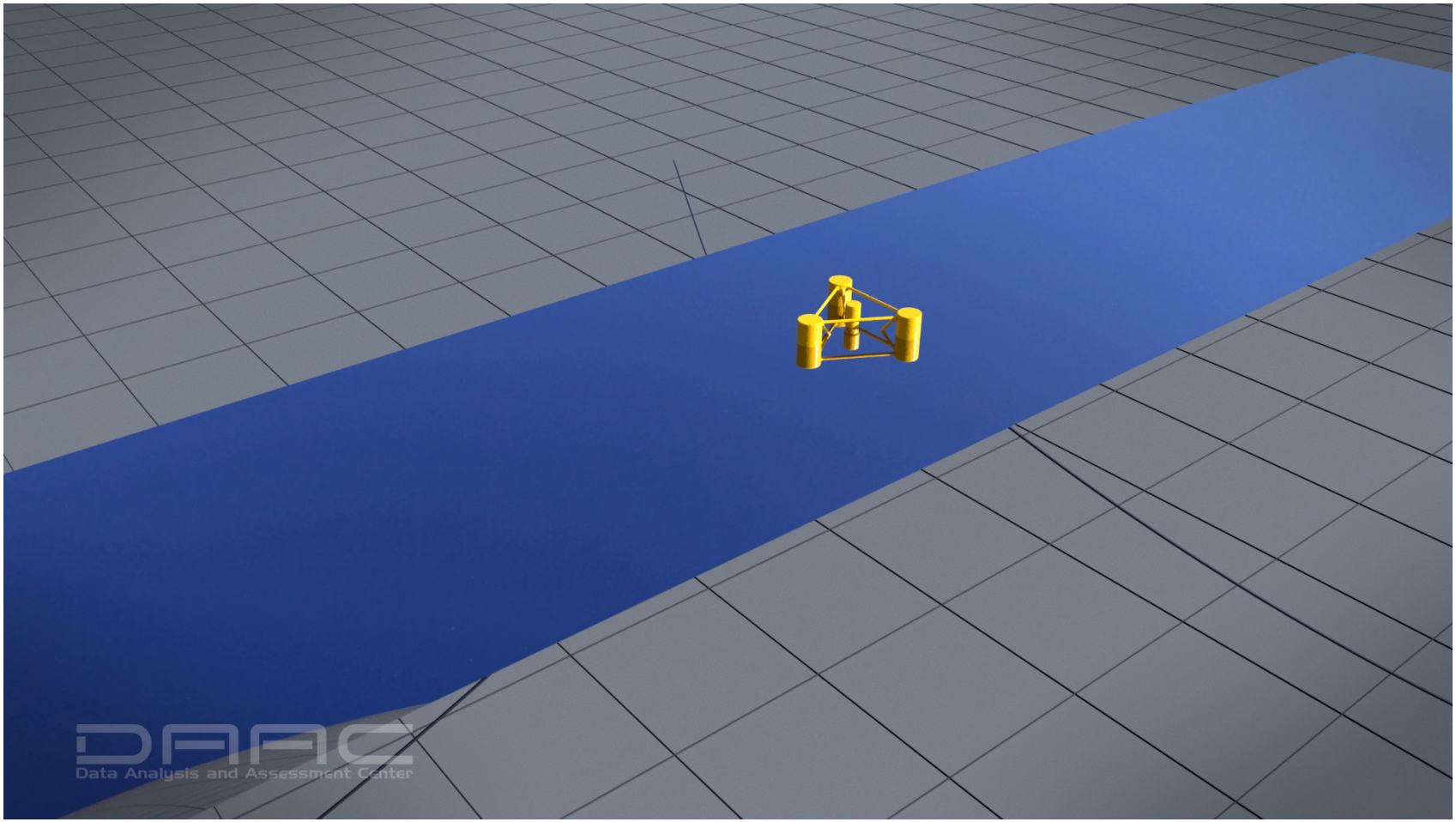
Computational Experiment: Offshore Platform



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Comparisons: Offshore Platform

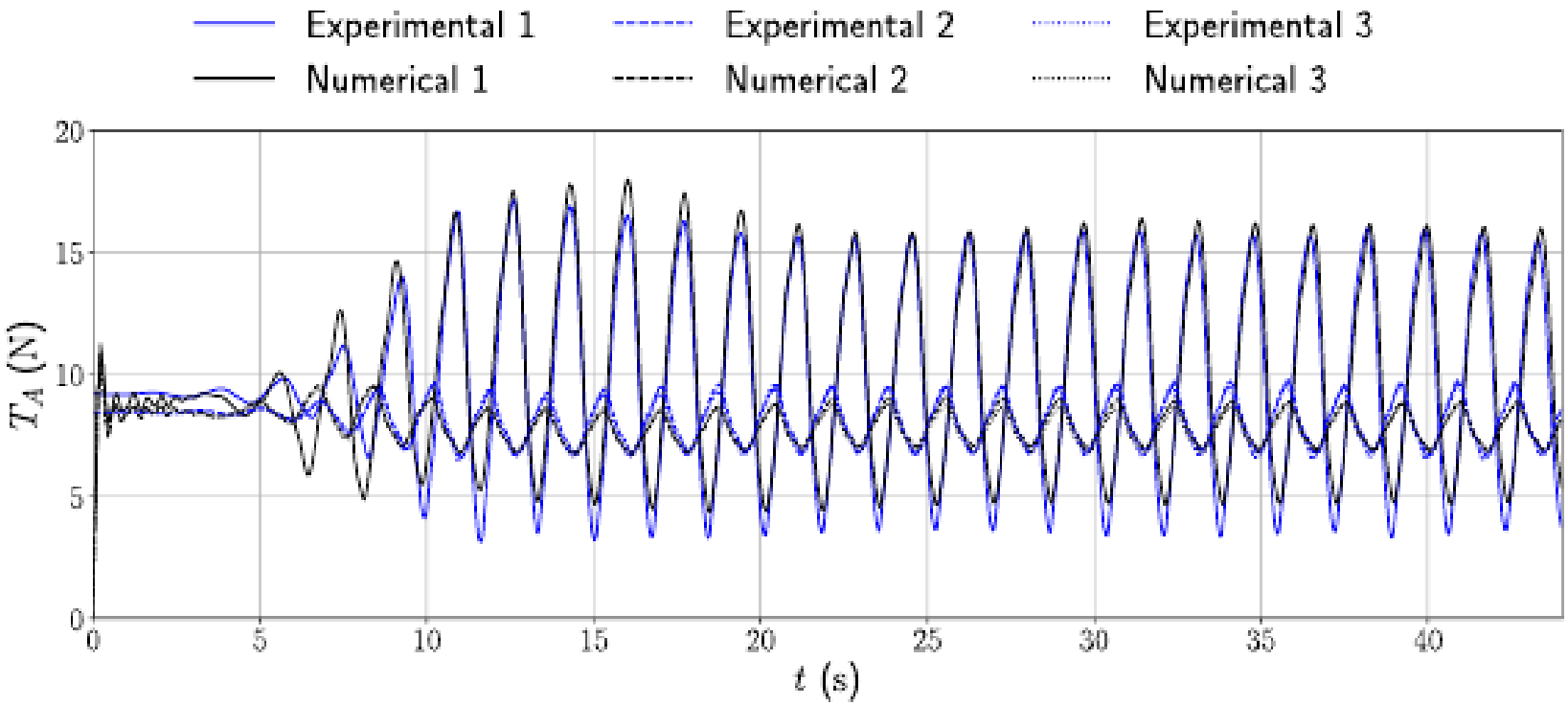


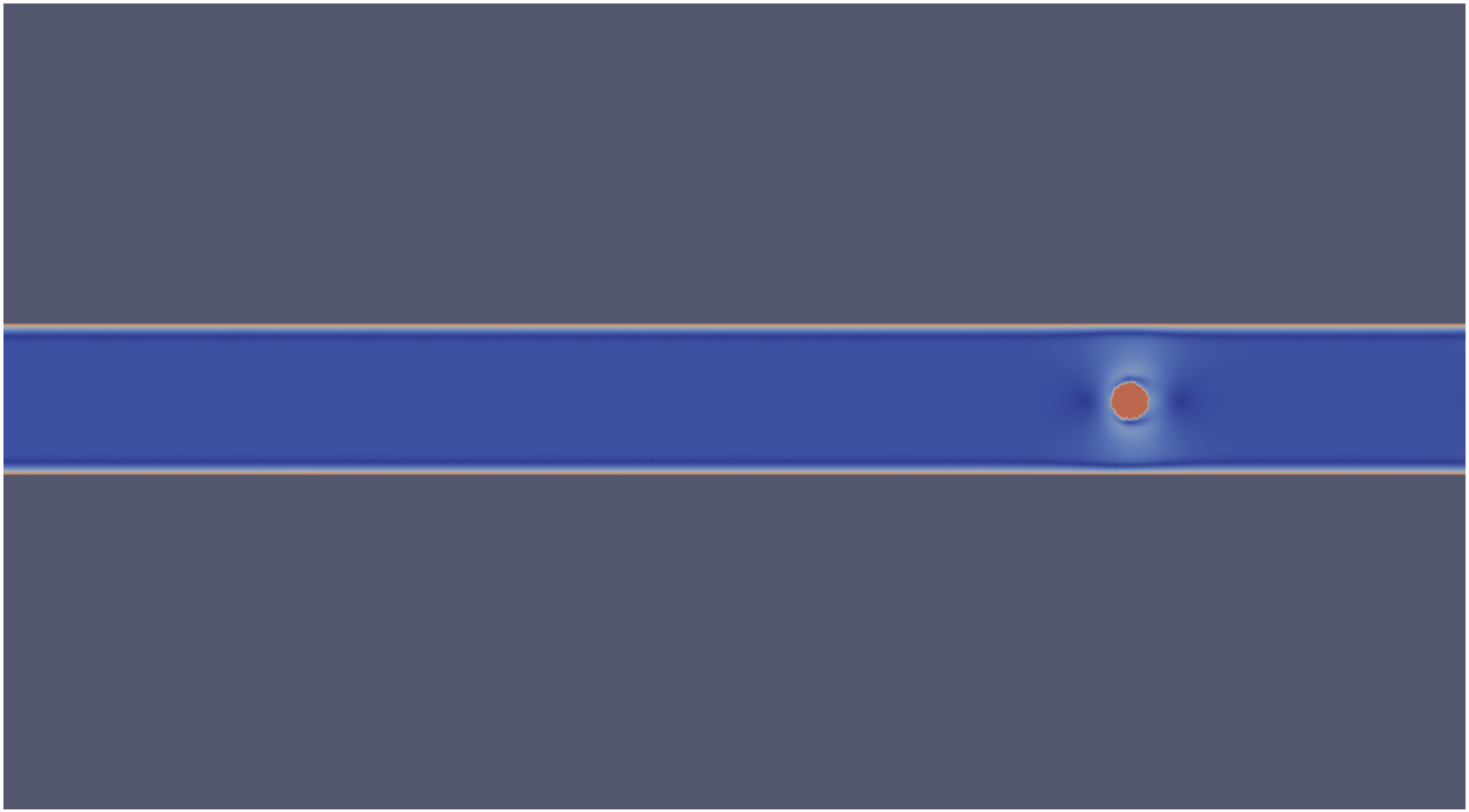
Figure V.39: Tensions at fairleads for coupled simulation of DeepCwind semi-submersible

Issues

- Strong mesh sensitivity of critical integral quantities, such as the drag and torque on particles.
- Difficulty resolving thin jets and related shear layers.
- Inability to preserve certain equilibrium states, such as flat water surface at hydrostatic pressure and zero velocity (lake at rest).

Hypothesis: These issues arise from the use of regularized Heaviside and Dirac functions to approximate integrals in cells cut by interfacial boundaries, leading to poor enforcement of interfacial jump conditions.
Approach: Integrate cut cells exactly and enforce proper jump conditions at interfaces.

Scripted Cylinder Test



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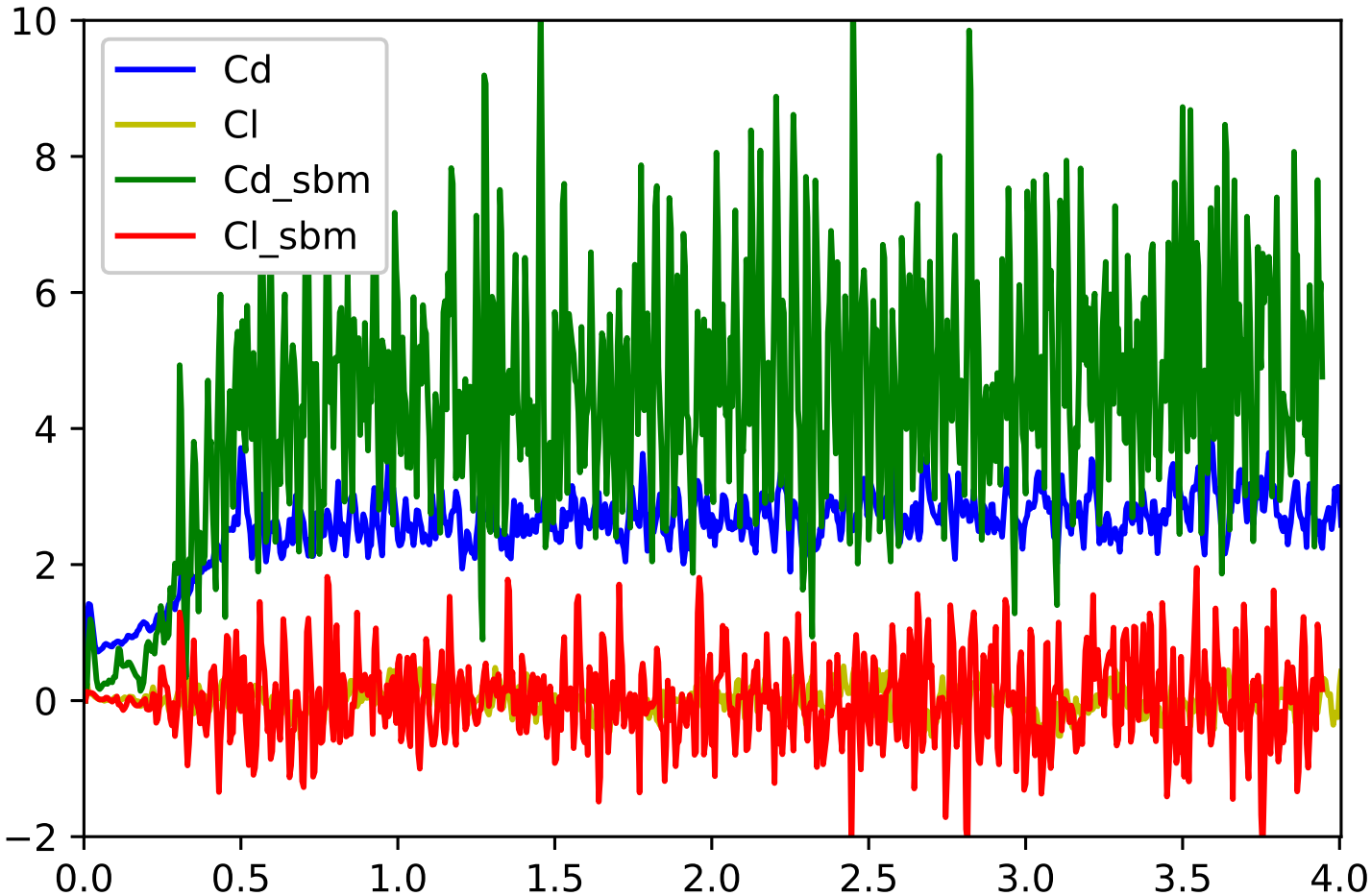
Force Oscillations for Moving Bodies



Solid Surface Area Oscillations

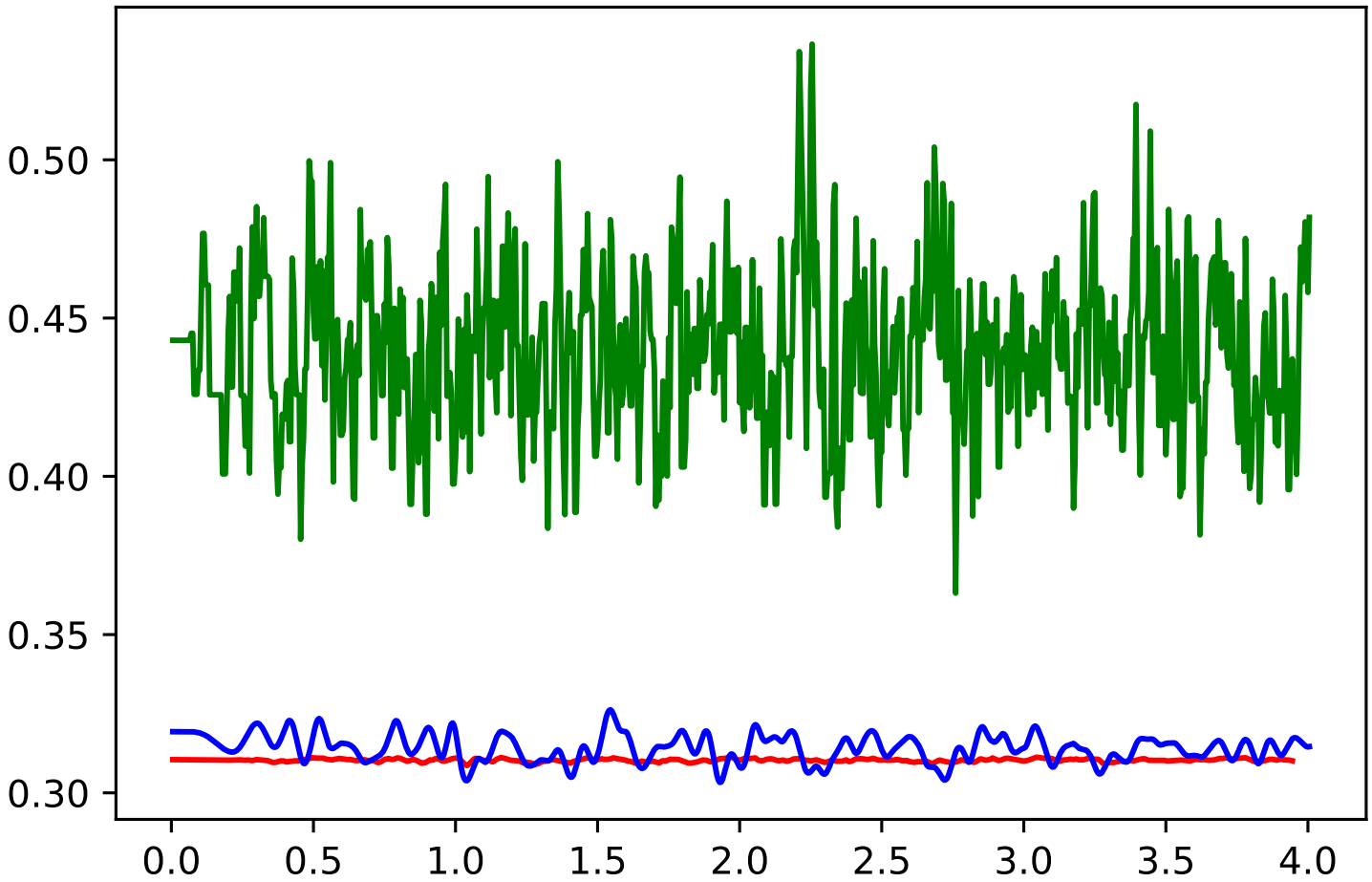


Figure: Green=SBM, Blue=IBM, Red=Cut

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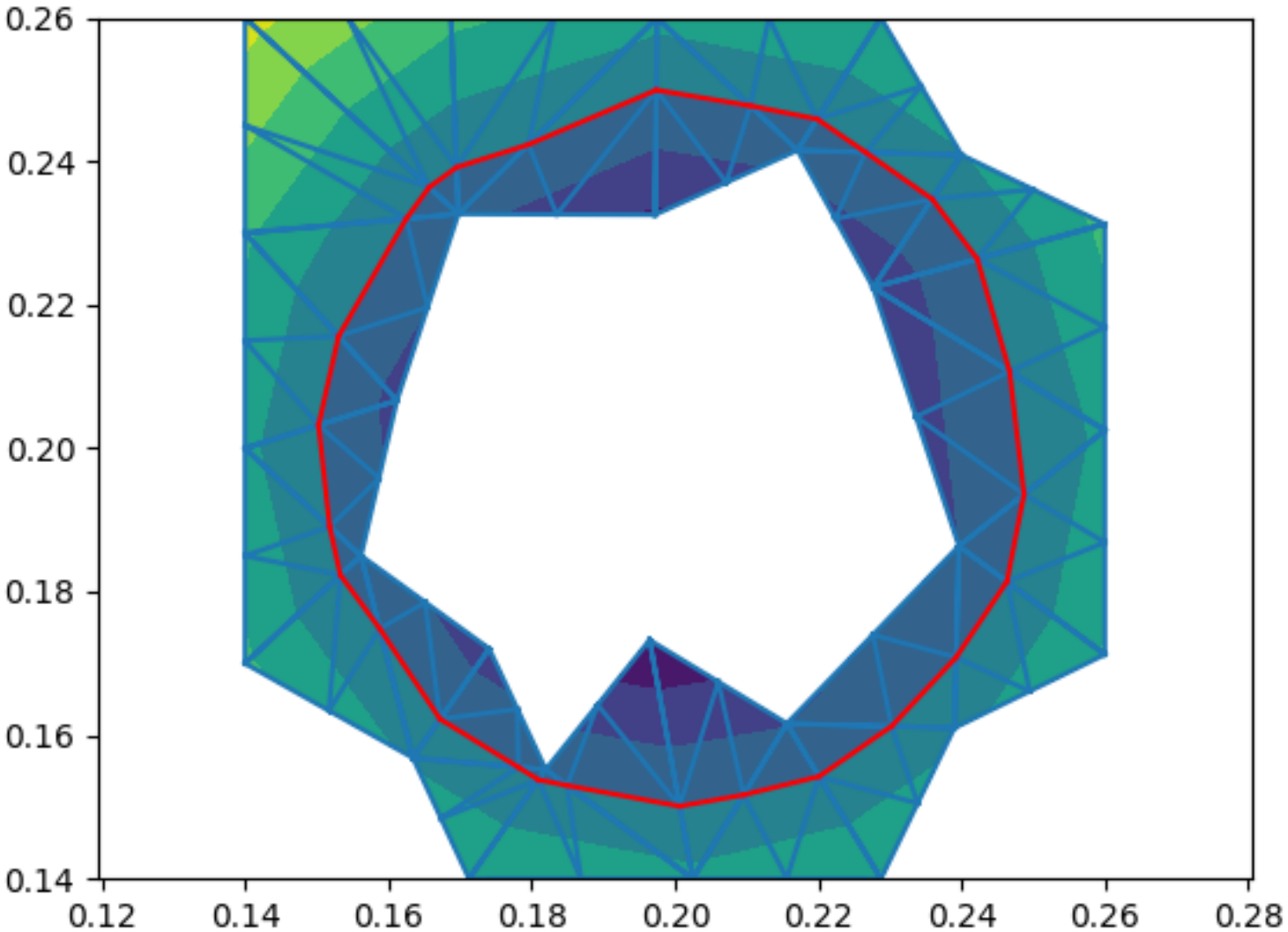
Cut Cell Integration



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Three Phase Formulation with Jump Conditions

$$\nabla \cdot \mathbf{u}_a = 0, \quad \text{in } \Omega_a \tag{1.6a}$$

$$\rho_a(\partial_t \mathbf{u}_a + (\mathbf{u}_a \cdot \nabla)\mathbf{u}_a) - \nabla \cdot \sigma_a = \rho_a \mathbf{g}, \quad \text{in } \Omega_a \tag{1.6b}$$

$$\nabla \cdot \mathbf{u}_w = 0, \quad \text{in } \Omega_w \tag{1.6c}$$

$$\rho_w(\partial_t \mathbf{u}_w + (\mathbf{u}_w \cdot \nabla)\mathbf{u}_w) - \nabla \cdot \sigma_w = \rho_w \mathbf{g}, \quad \text{in } \Omega_w \tag{1.6d}$$

$$\mathbf{u}_a - \mathbf{u}_w = 0 \quad \text{on } \Gamma_f \tag{1.6e}$$

$$\sigma_a \cdot \mathbf{n}_f - \sigma_w \cdot \mathbf{n}_f = \gamma \kappa \mathbf{n}_f \quad \text{on } \Gamma_f \tag{1.6f}$$

$$\sigma_a \cdot \mathbf{t}_{1,f} - \sigma_w \cdot \mathbf{t}_{1,f} = 0 \quad \text{on } \Gamma_f \tag{1.6g}$$

$$\sigma_a \cdot \mathbf{t}_{2,f} - \sigma_w \cdot \mathbf{t}_{2,f} = 0 \quad \text{on } \Gamma_f \tag{1.6h}$$

$$\mathbf{u} - \mathbf{u}_s = \mathbf{u}_c \quad \text{on } \Gamma_s \tag{1.6i}$$

$$\mathbf{u} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma \tag{1.6j}$$

where

$$\sigma = -pI + 2\mu\varepsilon(\mathbf{u}) \tag{1.7}$$

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Three-Phase Level Set Formulation

$$\int_{\Omega} H(\phi_s)\nabla\mathbf{v}\cdot\nabla\mathbf{w}dV = 0 \tag{1.8}$$

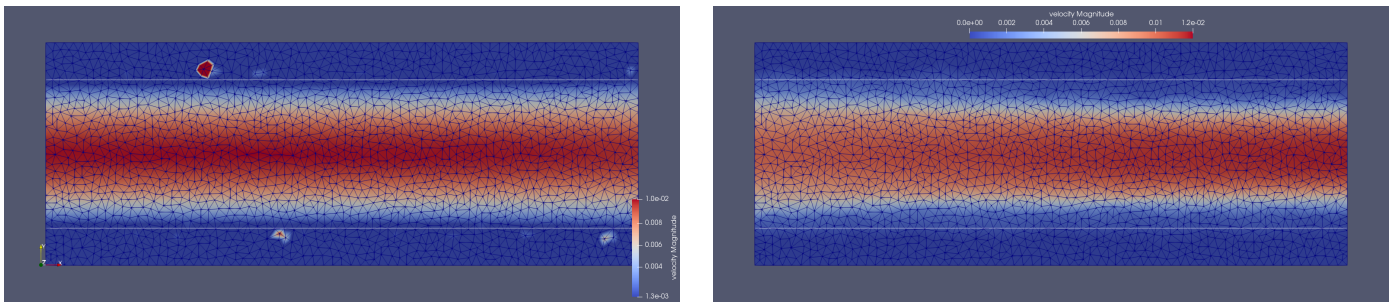
$$\int_{\Omega} H(\phi_s)\left\{\left[\rho\left(\frac{\partial\mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right)+\nabla p-\rho\mathbf{g}\right]\mathbf{w}+2\mu_f\varepsilon(\mathbf{v})\cdot\mathbf{w}\right\}dV$$
$$+\int_{\Omega}\delta(\phi_s)\left[-\mu(\phi)\frac{\partial\mathbf{v}}{\partial\mathbf{n}}\mathbf{w}-\mu(\phi)\frac{\partial\mathbf{w}}{\partial\mathbf{n}}\mathbf{v}+C(h_e)(\mathbf{v}-\mathbf{v}_s)\mathbf{w}\right]dV = 0 \tag{1.9}$$

CutFEM and Ghost Penalty

The coercivity of the problem needs to be extended to the computational domain. One approach is a an edge-based "Ghost Penalty"(Burman 2010).

$$j(u_h, v_h) := \sum_{F \in \mathcal{F}_G} \int_F [\gamma(\nabla u^+ - \nabla u^-) \cdot \mathbf{n}][(\nabla w^+ - \nabla w^-) \cdot \mathbf{n})] dS \tag{1.10}$$

where $\mathcal{F}_G$ is the set of internal element boundaries of cut cells.



CutFEM without ghost penalty (left) and with ghost penalty (right). See Massing, Schott, and Wall 2017 for Oseen/CIP.

Immersed Interface Finite Element Method (IIFEM)

- For two-fluid immersed interface problems, Leveque and Li developed a second order accurate finite difference scheme for by enforcing jump conditions for the solution and normal derivatives across the interface (LeVeque and Li 1994,1997)
- This approach was extended to FEM in the Immersed Interface Finite Element Method (IIFEM), by constructing a local basis with the desired jump conditions (Li et al. 2003, Ji et al. 2014)
- A key insight is that the algebraic system that results from doubling the number of degrees of freedom (as in CutFEM) leads to a solvable algebraic system for exactly half the duplicated degrees of freedom.

IIFEM Basis

Consider and elliptic immersed boundary problem with homogeneous jump conditions.

$$[u] = 0 \qquad [\mu \nabla u \cdot \mathbf{n}_f] = 0 \qquad \text{on } \Gamma_f \tag{1.11}$$

Consider one dimension where the cut element K is $(x_0, x_1) = (0, 1)$, $\Gamma_f = x_c \in (0, 1)$, and $\mathbf{n_f} = 1$. Define a new basis, ψ_0, ψ_1 on K by

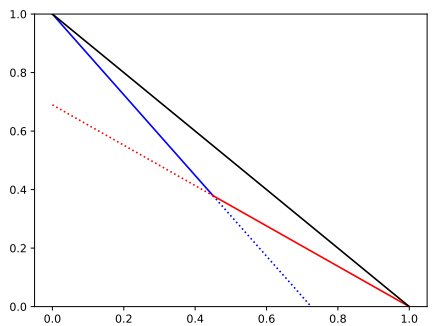
$$\psi_i = \begin{cases} \psi_i^a = a_1 + a_2 x & x \leq x_c \\ \psi_i^w = b_1 + b_2 x & x > x_c \end{cases} \tag{1.12}$$

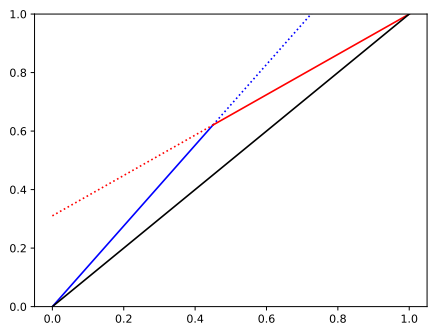
$$\psi_i^a(x_0) = \delta_{i0} \tag{1.13}$$

$$\psi_i^b(x_1) = \delta_{i1} \tag{1.14}$$

$$\psi_i^a(x_c) = \psi_i^b(x_c) \tag{1.15}$$

$$\mu_a \nabla \psi_i^b \cdot \mathbf{n}_f = \mu_w \nabla \psi_i^b \cdot \mathbf{n}_f \tag{1.16}$$





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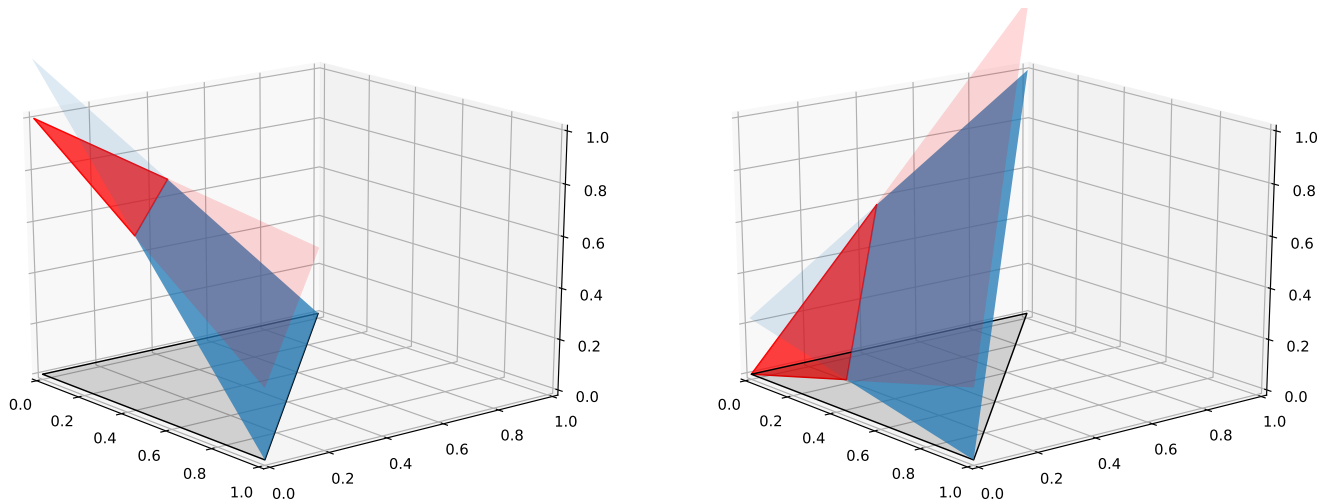
2D Basis functions



IIFEM basis functions (solid red/blue) for $\mu_w/\mu_a = 2$.

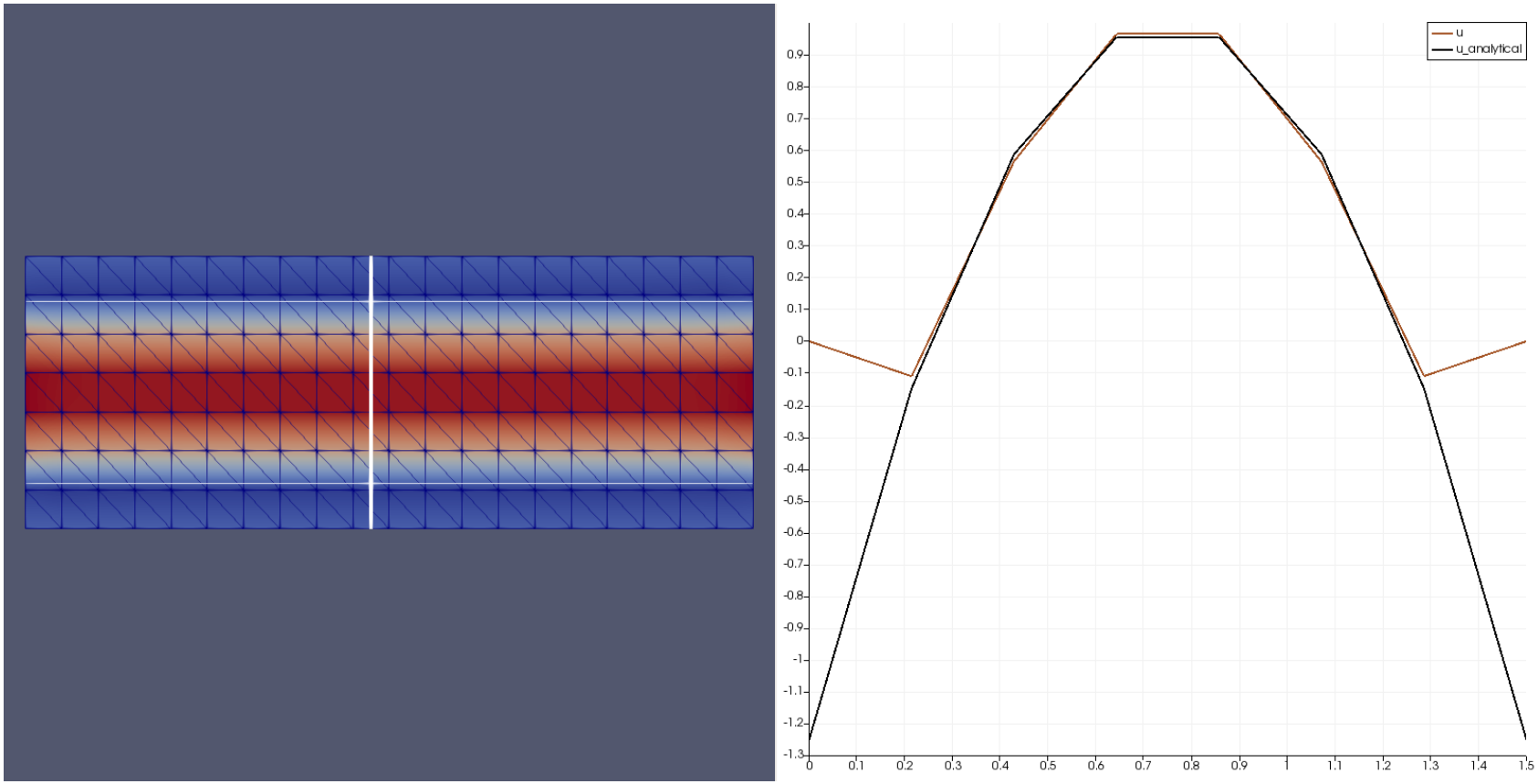
Cut Cell Integration by Equivalent Polynomials

- CutFEM and IIFEM introduce cut cells, which are challenge to integrate.
- Ventura and Bienvenuti 2015 introduced and approach based on generating “equivalent polynomial” Heaviside functions $\hat{H}$:

$$\int_K \hat{H} v_i = \int_K H v_i \quad i = 1, \ldots, \dim(P^m(K)) \tag{1.17}$$

  where $\hat{H}$ is also a polynomial of degree m.
- The FEM assembly then can proceed as if there were no cut cells as long as quadrature is sufficiently accurate.

CutFEM+Equivalent Polynomials: Duct



CutFEM + Equivalent Polynomials: Duct

Boundary Fitted Mesh

$\|(p-p^*)\|_1$	rate	$\|(u-u^*)\|_1$	rate
2.227590e-01	-	1.363730e-01	-
6.441190e-02	1.79	3.134070e-02	2.12
1.763730e-02	1.87	7.534600e-03	2.06
4.577860e-03	1.95	1.846190e-03	2.03
1.166740e-03	1.97	4.568420e-04	2.01
$\|(p-p^*)\|_2$	rate	$\|(u-u^*)\|_2$	rate
3.653670e-01	-	7.759540e-02	-
1.414790e-01	1.37	1.734230e-02	2.16
4.869300e-02	1.54	4.120990e-03	2.07
1.673540e-02	1.54	1.004600e-03	2.04
5.808630e-03	1.53	2.479960e-04	2.02
$\|(p-p^*)\|_\infty$	rate	$\|(u-u^*)\|_\infty$	rate
1.265980e+00	-	5.876160e-02	-
6.661940e-01	0.93	1.242080e-02	2.24
3.307870e-01	1.01	2.927460e-03	2.09
1.639120e-01	1.01	7.119360e-04	2.04
8.155440e-02	1.01	1.755150e-04	2.02

Unfitted Mesh

$\|(p-p^*)\|_1$	rate	$\|(u-u^*)\|_1$	rate
4.889190e-01	-	1.185600e-01	-
1.302270e-01	1.91	3.219830e-02	1.88
2.783510e-02	2.23	7.328950e-03	2.14
7.202650e-03	1.95	1.811790e-03	2.02
1.840000e-03	1.97	4.503920e-04	2.01
$\|(p-p^*)\|_2$	rate	$\|(u-u^*)\|_2$	rate
4.405330e-01	-	6.659730e-02	-
2.406210e-01	0.87	1.774190e-02	1.91
6.604950e-02	1.87	4.018790e-03	2.14
2.304690e-02	1.52	9.873070e-04	2.03
8.097610e-03	1.51	2.447100e-04	2.01
$\|(p-p^*)\|_\infty$	rate	$\|(u-u^*)\|_\infty$	rate
1.120820e+00	-	5.373470e-02	-
1.353560e+00	-0.27	1.586260e-02	1.76
3.435390e-01	1.98	3.038940e-03	2.38
1.786160e-01	0.94	7.363010e-04	2.05
9.701790e-02	0.88	1.817440e-04	2.02

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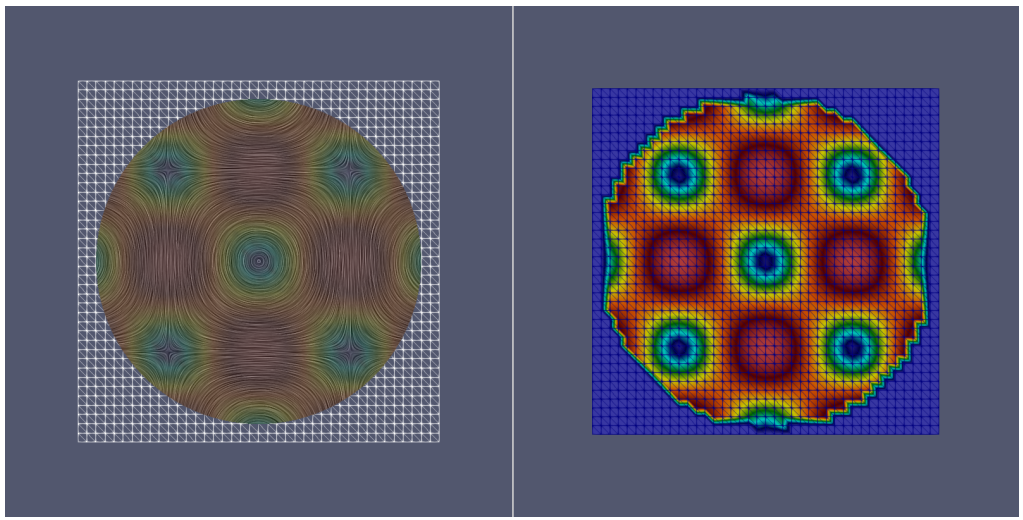
CutFEM + Equivalent Polynomials: Taylor

Boundary Fitted Mesh

$\|(p-p^*)\|_1$	rate	$\|(u-u^*)\|_1$	rate
1.629910e-01	-	4.533020e-03	-
6.031340e-02	1.43	1.693180e-03	1.42
1.619510e-02	1.90	4.778660e-04	1.83
4.442810e-03	1.87	1.332800e-04	1.84
$\|(p-p^*)\|_2$	rate	$\|(u-u^*)\|_2$	rate
5.041250e-01	-	7.002600e-03	-
2.233220e-01	1.17	2.642520e-03	1.41
7.756350e-02	1.53	7.476140e-04	1.82
2.782230e-02	1.48	2.086930e-04	1.84
$\|(p-p^*)\|_\infty$	rate	$\|(u-u^*)\|_\infty$	rate
3.546620e+00	-	2.181050e-02	-
2.054580e+00	0.79	8.358510e-03	1.38
1.010460e+00	1.02	2.662330e-03	1.65
5.080040e-01	0.99	7.365010e-04	1.85

Unfitted Mesh

$\|(p-p^*)\|_1$	rate	$\|(u-u^*)\|_1$	rate
4.650280e-01	-	1.605080e-02	-
1.864090e-01	1.32	4.886610e-03	1.72
5.555430e-02	1.75	1.363970e-03	1.84
1.479990e-02	1.91	3.573620e-04	1.93
$\|(p-p^*)\|_2$	rate	$\|(u-u^*)\|_2$	rate
9.362260e-01	-	2.542980e-02	-
4.430540e-01	1.08	7.362900e-03	1.79
1.672410e-01	1.41	2.016140e-03	1.87
5.911910e-02	1.50	5.260030e-04	1.94
$\|(p-p^*)\|_\infty$	rate	$\|(u-u^*)\|_\infty$	rate
5.842120e+00	-	7.515420e-02	-
3.669590e+00	0.67	2.067450e-02	1.86
1.910150e+00	0.94	5.335560e-03	1.95
9.799620e-01	0.96	1.349950e-03	1.98



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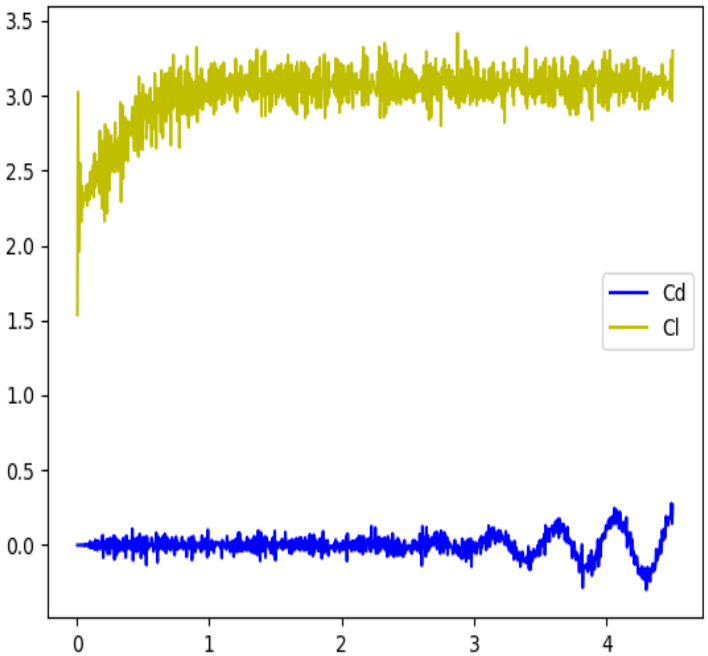
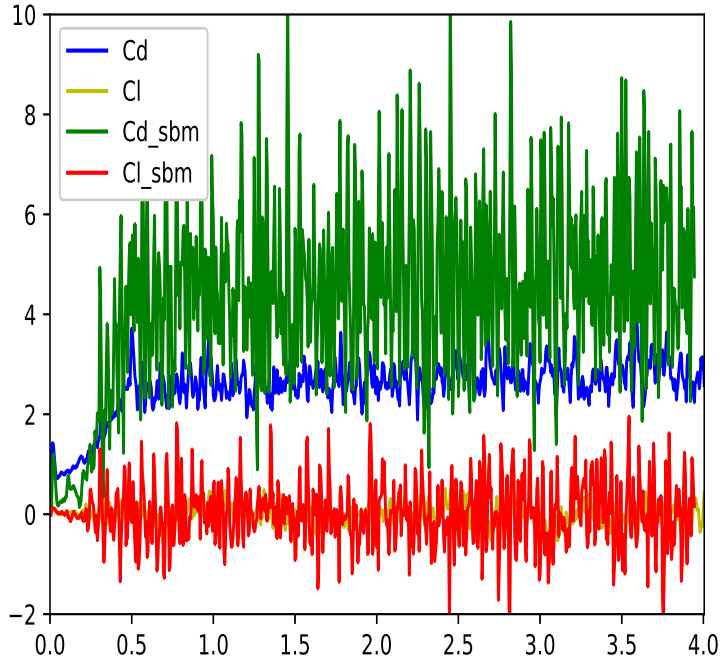
CutFEM + Equivalent Polynomials: Falling Cylider





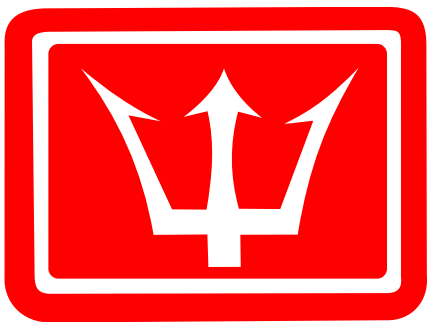
Future Work

- Use a more careful discretization of the fluid material derivative near the moving solid interface or space-time FEM.
- Compare to the aggregated unfitted approach of Badia, Verdugo, and Martin (2018) and investigate EQP-based implementation.
- Complete the IIFEM implementation for air/water and investigate whether it removes various numerical artifacts.
- Deal with three-phase cutcells and contact line boundary conditions.

Software Challenges

- Bridge “valley of death” between new advancements in model formulations/numerics and production codes/applications.
- Break out of the “model trap” in which R&D is stovepiped around a single set of equations or single method.
- Explicit multi-physics and multi-numerics support.

“Good numerics is ultimately about getting things to work; the slavish and blind devotion to one approach above all others is usually a sign of unfamiliarity with the range of troubles and challenges presented by real applications.” -James Sethian



Proteus Toolkit
Source code
https://github.com/erdc/proteus

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What is Proteus?

- Proteus is a Python package for rapidly developing computer models and numerical methods.
- The package contains a collection of modules implemented in C,C++,Fortran, and Python.
- We try to separate the physics implementation and numerical methods implementation.
- Has a layered API for model implementation. Highly optimized models for specific/detailed physics can be implemented by deriving from more generic models.
- Works with many 3rd party tools: PETSc, Trilinos, Chrono, triangle, tetgen, gmsh, scipy, sympy...

Equations Solved

- 2D & 3D incompressible Navier-Stokes (Unsteady/Steady, LES, RANS, VANS)
- 2D diffusive wave (overland flow)
- 2D shallow water and Green-Naghdi (dispersive shallow water)
- 2D & 3D two-phase incompressible, immiscible flow (hybrid VOF/level set formulation with LES, etc.)
- 2D & 3D saturated groundwater
- 2D & 3D Richards' equation (variably saturated groundwater, various constitutive models)
- 2D & 3D two-phase flow in porous media (continuum mixture formulation, incompressible or compressible)
- 2D & 3D density-dependent groundwater flow and salinity transport
- 2D & 3D eikonal equation (signed distance calculations)
- 3D elastoplastic deformation (levee stability, Mohr-Coulomb material)
- 2D & 3D 6DOF solid/air/water interaction

Verified Numerics

- Continuous linear and quadratic polynomial spaces (C^0P^1 and C^0P^2) on simplicial elements (intervals, triangles, tetrahedra) with nodal (Lagrange) basis and Bernstein basis.
- Continuous tensor product spaces (C^0Q^k) on hex/quad
- Discontinuous complete polynomial spaces ($C^{-1}P^k$) on simplicial elements with monomial basis
- P^1 non-conforming simplicial elements
- Locally discontinuous Galerkin mixed elements with static condensation
- SIPG/NIPG/IIPG primal discontinuous elements
- Residual-based variational multiscale methods (RBVMS)
- Entropy viscosity, algebraic stabilization, and FCT
- Analytical Riemann solvers (numerical fluxes) for linear advection, two-phase flow in porous media, and shallow water
- Approximate Riemann solvers: Harten-Lax-van Leer (SWE), Rusanov (two-phase flow), Cheng-Shu (Hamilton-Jacobi)
- Velocity post-processing to enforce element-wise (local) conservation

Popular Modeling Toolkit for PDE's

- "The COMSOL multiphysics simulation environment facilitates all steps in the modeling process: defining your geometry, specifying your physics, meshing, solving and then post-processing your results."
- "FEniCS is free software for automated solution of differential equations. We provide software tools for working with computational meshes, finite element variational formulations of PDEs, ODE solvers and linear algebra."
- "...OpenFOAM is a flexible set of efficient C++ modules. These are used to build a wealth of: solvers, to simulate specific problems in engineering mechanics; utilities, to perform pre- and post-processing tasks ranging from simple data manipulations to visualization and mesh processing; libraries, to create toolboxes that are accessible to the solvers/utilities, such as libraries of physical models."

Second Order Nonlinear, Heterogeneous Transport Systems

Our target problems are systems of nonlinear equations governing the transport of an abstract vector of components $u_j, j = 1, \ldots, n_c$:

$$\frac{\partial m^i}{\partial t} + \nabla \cdot \left(\mathbf{f}^i - \sum_k^{n_c} \boldsymbol{a}^{ik} \nabla \phi^k \right) + r^i + h^i(\nabla u) = 0$$

where $i = 1, \ldots n_c$. The large majority of models in hydrology, hydraulics, and coastal engineering are in this class.

A simple example

For $(t, x, y) \in [0, T] \times [0, 1] \times [0, 1]$ find u such that

$$
\begin{aligned}
(Mu)_t + \nabla \cdot [\mathbf{B}u - \boldsymbol{A}\nabla u] &= 0 \\
u(0, x, y) &= 0 \\
u(t, x, 0) &= u(t, 0, y) = 1 \\
u(t, x, 1) &= u(t, 1, x) = 0 \\
M &= 1 \\
\mathbf{B} &= (1, 1) \\
\boldsymbol{A} &= 0.001\boldsymbol{I}
\end{aligned}
$$

adr.py

```
20      def evaluate(self,t,c):
21          c[('m',0)][:]           = self.M*c[('u',0)]
22          c[('dm',0,0)][:]        = self.M
23          c[('f',0)][...,0]       = self.B[0]*c[('u',0)]
24          c[('f',0)][...,1]       = self.B[1]*c[('u',0)]
25          c[('df',0,0)][...,0]    = self.B[0]
26          c[('df',0,0)][...,1]    = self.B[1]
27          c[('a',0,0)][...,0] = self.A[0][0]
28          c[('a',0,0)][...,3] = self.A[1][1]
```

adr.py

```
3  class LAD(TC_base):
4      """
5      Coefficients for linear advection-diffusion
6      """
7      def __init__(self,M,A,B):
8          TC_base.__init__(self,
9                           nc=1, #number of components
10                          variableNames=['u'],
11                          mass      = {0:{0:'linear'}},
12                          advection = {0:{0:'linear'}},
13                          diffusion = {0:{0:{0:'constant'}}},
14                          potential = {0:{0:'u'}},
15                          reaction  = {0:{0:'linear'}})
16         self.M=M;
17         self.A=A;
18         self.B=B;
19
20     def evaluate(self,t,c):
```

ladr_2d_p.py

```
6   nd = 2; #Two dimensions
7   L=(1.0,1.0,1.0);
8   T=1.0
9
10  coefficients=LAD(M=1.0,
11                   A=[[0.001,0.0],
12                      [0.0,0.001]],
13                   B=[2.0,1.0])
14
15  def getDBC(x,flag):
16      if x[0] == 0.0 or x[1] == 0.0:
17          return lambda x,t: 1.0
18      elif x[0] == 1.0 or x[1] == 1.0:
19          return lambda x,t: 0.0
20
21  dirichletConditions = {0:getDBC}
22  advectiveFluxBoundaryConditions = {}
23  diffusiveFluxBoundaryConditions = {0:{}}
```

ladr_2d_c0p2_n.py

```
4  timeIntegration = BackwardEuler
5  femSpaces = {0:C0_AffineQuadraticOnSimplexWithNodalBasis}
6  elementQuadrature = SimplexGaussQuadrature(nd,5)
7  elementBoundaryQuadrature = SimplexGaussQuadrature(nd-1,5)
8  nnx=11; nny=11
9  nLevels=1
10 tnList=[float(i)/10.0 for i in range(11)]
11 matrix = SparseMatrix
12 multilevelLinearSolver = LU
13 subgridError = AdvectionDiffusionReaction_ASGS(coefficients,
14                                                nd)
15 shockCapturing = ResGradQuad_SC(coefficients,
16                                  nd,
17                                  shockCapturingFactor=0.9,
18                                  lag=True)
```

A multi-physics example

```
1  pnList = [("twp_navier_stokes_sloshbox_2d_p" ,
2             "twp_navier_stokes_sloshbox_2d_c0p1c0p1_n"),
3            ("ls_sloshbox_2d_p" ,
4             "ls_sloshbox_2d_c0p1_n"),
5            ("vof_sloshbox_2d_p" ,
6             "vof_sloshbox_2d_c0p1_n"),
7            ("redist_sloshbox_2d_p" ,
8             "redist_sloshbox_2d_c0p1_n"),
9            ("ls_consrv_sloshbox_2d_p" ,
10            "ls_consrv_sloshbox_2d_c0p1_n")]
```

Domain Specific Languages

- DSL's have proven useful linear algebra (FLAME), and FEM (FEniCS, Firedrake)
- Representing PDE's in continuous, strong formulation as classes allows modular backends for fully discrete formulations (FEM, FVM, FDM,...)
- With a DSL, information can be inferred from a suitable symbolic expression (and potentially optimized) and the API code can be generated.
- As a proof of concept we developed a simpled Domain Specific Language embedded in Python based on pymbolic (with A. Klöckner, Illinois and R. Kirby, Baylor)
- Earlier attempts include an embedded LaTeX DSL [Farthing, Sassen, Prins, Miller, 2004]

DSL: Burgers

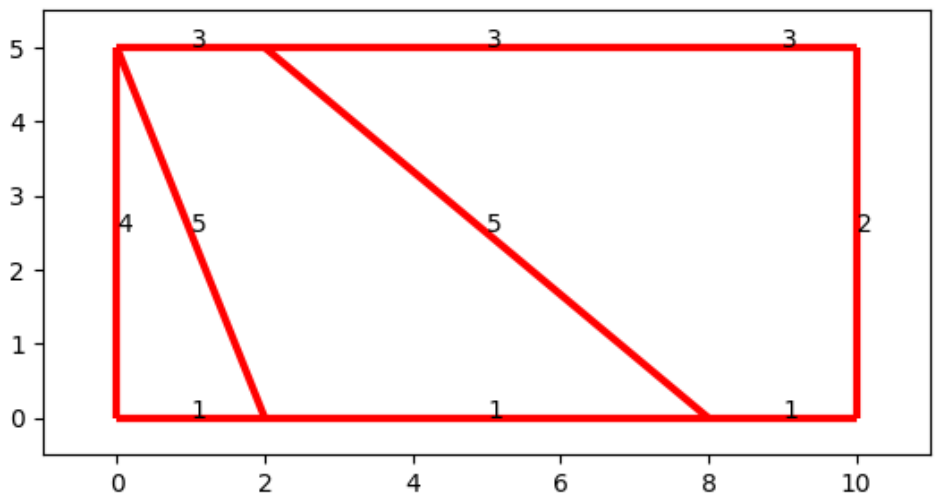
```
6
7   A = 1.0e-1
8   B = np.array([1.0, 2.0])
9   C = 1.0e-12
10
11  u = sym.Field("u")
12  eqns = sym.join(sym.d_dt(u)
13                  + sym.div(B * u**2)
14                  - sym.div(A*sym.grad(u))
15                  + C*u)
16
17  coefficients = generate_coefficients(eqns,
18                                       unknowns=[u],
19                                       dim=2,
20                                       name="Burgers")
21
```

PDE Domains

- Defining the PDE represents only a small fraction of the work for real applications.
- Precisely defining the domain geometry, material properties, boundary conditions, and obtaining good quality meshes is frequently a stumbling block–we aren't taught this in class.

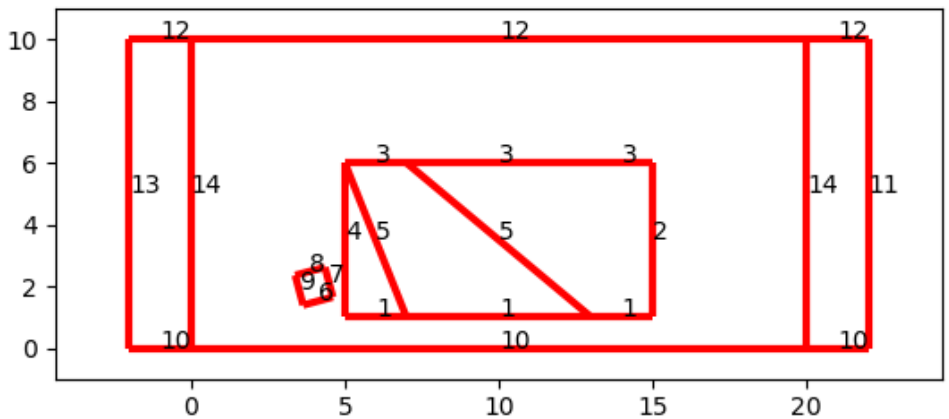
SpatialTools: Shapes

```
1   domain2D = Domain.PlanarStraightLineGraphDomain()
2
3   vertices = [[0., 0.], [2., 0.], [8., 0.], [10., 0.],
4               [10., 5.], [8., 5.], [2., 5.], [0., 5.]]
5   segments = [[0, 1], [1, 2], [2, 3], [3, 4],
6               [4, 5], [5, 6], [6, 7], [7, 0],
7               [1, 7], [2, 6]]
8
9   bt = {'bottom': 1, 'right': 2, 'top': 3, 'left': 4, 'sponge': 5}
10  vertexFlags = [bt['bottom'], bt['bottom'], bt['bottom'], bt['bottom'],
11                 bt['top'], bt['top'], bt['top'], bt['top'],
12                 bt['sponge'], bt['sponge']]
13  segmentFlags = [1, 1, 1, 2, 3, 3, 3, 4, 5, 5]
14  regions = [[1., 1.], [5., 1.], [9., 1.]]
15  regionFlags = [2, 1, 3]
16
17  custom = st.CustomShape(domain2D, boundaryTags=bt,
18                          vertices=vertices, vertexFlags=vertexFlags,
19                          segments=segments, segmentFlags=segmentFlags,
20                          regions=regions, regionFlags=regionFlags)
```



SpatialTools: Modification and Composition

```
22  custom.translate([5., 1.])
23
24  tank = st.Tank2D(domain2D, dim=[20., 10.])
25  tank.setSponge(x_n=2., x_p=2.)
26
27  rectangle = st.Rectangle(domain2D, dim=[1., 1.], coords=[2., 2.])
28  rectangle.rotate(np.pi/12., pivot=[2., 2.])
29  rectangle.setBarycenter(my_rectangle.coords)
30  rectangle.setPosition([4., 2.])
31  st.assembleDomain(domain2D)
```



Numerical Methods R&D

- Convervative level set schemes for FEM
  - Incompressible Two-phase Flow via a Monolithic Phase-Conservative Level Set Method (2019) M.Quezada de Luna, J.H. Collins, and C.E. Kees *International Journal for Numerical Methods in Fluids*, In Review, https://arxiv.org/abs/1903.06919.
  - A Monolithic Conservative Level Set Method with Built-In Redistancing (2019) M. Quezada de Luna, D. Kuzmin, C.E. Kees, *Journal of Computational Physics*, 379, 262-278, https://doi.org/10.1016/j.jcp.2018.11.044
  - A Conservative Level Set Method for Variable-Order Approximations and Unstructured Meshes (2011) C.E. Kees, I. Akkerman, Y. Bazilevs, and M.W. Farthing. *Journal of Computational Physics*, 230(12), 4536–4558, https://doi.org/10.1016/j.jcp.2011.02.030.
- Equivalent polynomials for exact Heaviside and Dirac integrals with IIFEM (In progress)
- Fluid-structure interaction with ALE, added mass stabilization, and $h-$adaptivity
  - High-Fidelity Computational Modelling of Fluid-Structure Interaction for Moored Floating Bodies (2019) T. de Lataillade *Doctoral Thesis, Edinburgh/Exeter/Strathcylde*
  - Dynamic, Anisotropic Adaptive Mesh Refinement for Fluid-Structure Interaction (2019) A. Zhang *Doctoral Thesis, RPI*.

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Numerical Methods R&D, Cont'd

- Entropy viscosity methods for subgrid/numerical viscosity
  - Robust and Explicit Relaxation Technique for Solving the Green-Naghdi Equations (2019) J.-L. Guermond, B. Popov, E. Tovar, and C.E. Kees *Journal of Computational Physics*, In Press.
  - Well-Balanced Second-Order Finite Element Approximation of the Shallow Water Equations with Friction (2018) J.L. Guermond, M.Q. de Luna, B. Popov, C.E. Kees, and M.W. Farthing *SIAM Journal on Scientific Computing* 40(6), A3873-A3901,https://doi.org/10.1137/17M1156162.
- Scalable preconditioners based on multi-phase extensions of the pressure convection-diffusions approximation of the Schur complement.
  - Preconditioners for Two-Phase Incompressible Navier-Stokes Flow (2019) N. Bootland, C.E. Kees, A. Wathen, A. Bentley *SIAM Journal on Scientific Computing*, 41(4), B843–B869, https://doi.org/10.1137/17M1153674.
- Model Reduction (POD and PR-RBC)
  - Evaluation of Galerkin and Petrov-Galerkin Model Reduction for Finite Element Approximations of the Shallow Water Equations (2017) A. Lozovsky, M. W. Farthing, and C.E. Kees *Computational Methods in Applied Mechanics and Engineering* 318, 537-571, https://doi.org/10.1016/j.cma.2017.01.027
  - POD-Based Model Reduction for Stabilized Finite Element Approximations of Shallow Water Flows (2016) A. Lozovskiy, M.W. Farthing, C.E. Kees, E. Gildin *Journal of Computational and Applied Mathematics*, 302, 50-70, https://doi.org/10.1016/j.cam.2016.01.029.

Modeling and Engineering Applications

- Waves and structures
  - Fast Random Wave Generation in Numerical Tanks (2019) A. Dimakopoulos, T. de Lataillade, C.E. Kees, *Engineering and Computational Mechanics*, *Proceedings of the Institution of Civil Engineers - Engineering and Computational Mechanics*, 1-29, https://doi.org/10.1680/jencm.17.00016.
  - Simulating Oscillatory and Sliding Displacements of Caisson Breakwaters Using a Coupled Approach (2019) G. Cozzuto, A. Dimakopoulos, T. de Lataillade, P.O. Morillas, and C.E. Kees, *Journal of Waterway, Port, Coastal, and Ocean Engineering*, 145(3), p.04019005, https://doi.org/10.1061/(ASCE)WW.1943-5460.0000504
  - Computational Model for Wave Attenuation by Flexible Vegetation (2018) S.A. Mattis, C.E. Kees, M.V. Wei, A. Dimakopoulos, and C.N. Dawson, *Journal of Waterway, Port, Coastal, and Ocean Engineering* 145(1), p.04018033, https://doi.org/10.1061/(ASCE)WW.1943-5460.0000487
  - An Immersed Structure Approach for Fluid-Vegetation Interaction (2015) S.A. Mattis, C.N. Dawson, C.E. Kees, M.W. Farthing, *Advances in Water Resources*, 80,1-16, https://doi.org/10.1016/j.advwatres.2015.02.014.
- Three-dimensional sediment processes
  - Modeling Sediment Transport in Three-Phase Surface Water Systems (2019) C.T. Miller, W.G. Gray, C.E. Kees, I.V. Rybak, B.J. Shepherd, *Journal of Hydraulic Engineering*, https://doi.org/10.1080/00221686.2019.1581673.
  - Thermodynamically Constrained Averaging Theory: Principles, Model Hierarchies, and Deviation Kinetic Energy Extensions (2018) C.T. Miller, W. G. Gray, and C. E. Kees *Entropy* 20(4), 253, https://doi.org/10.3390/e20040253
- Water resources
  - Finite Element Methods for Variable Density Flow And Solute Transport (2013) T.J. Povich, C.N. Dawson, M.W. Farthing, C.E. Kees *Computational Geosciences* 17(3), 529-549, https://doi.org/10.1007/s10596-012-9330-2.
  - Numerical Simulation of Water Resources Problems: Models, Methods, and Trends (2013) C.T. Miller, C.N. Dawson, M.W. Farthing, T.Y. Hou, J. Huang, C. E. Kees, C.T. Kelley, and H.P. Langtangen *Advances in Water Resources*, 51, 405-437, https://doi.org/10.1016/j.advwatres.2012.05.008

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Thank You!

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