JAX-SPH
A Differentiable Smoothed Particle Hydrodynamics Framework

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TL;DR

JAX-SPH is a Smoothed Particle Hydrodynamics (SPH) framework implemented in JAX. JAX-SPH extends the code for dataset generation from the LagrangeBench project [Toshev et al., 2024] by: (a) integrating **further key SPH algorithms**, (b) restructuring the code toward a **Python package**, (c) validating solver gradients numerically, and (d) showcasing **machine learning applications of the differentiable solver**.

SPH Solver

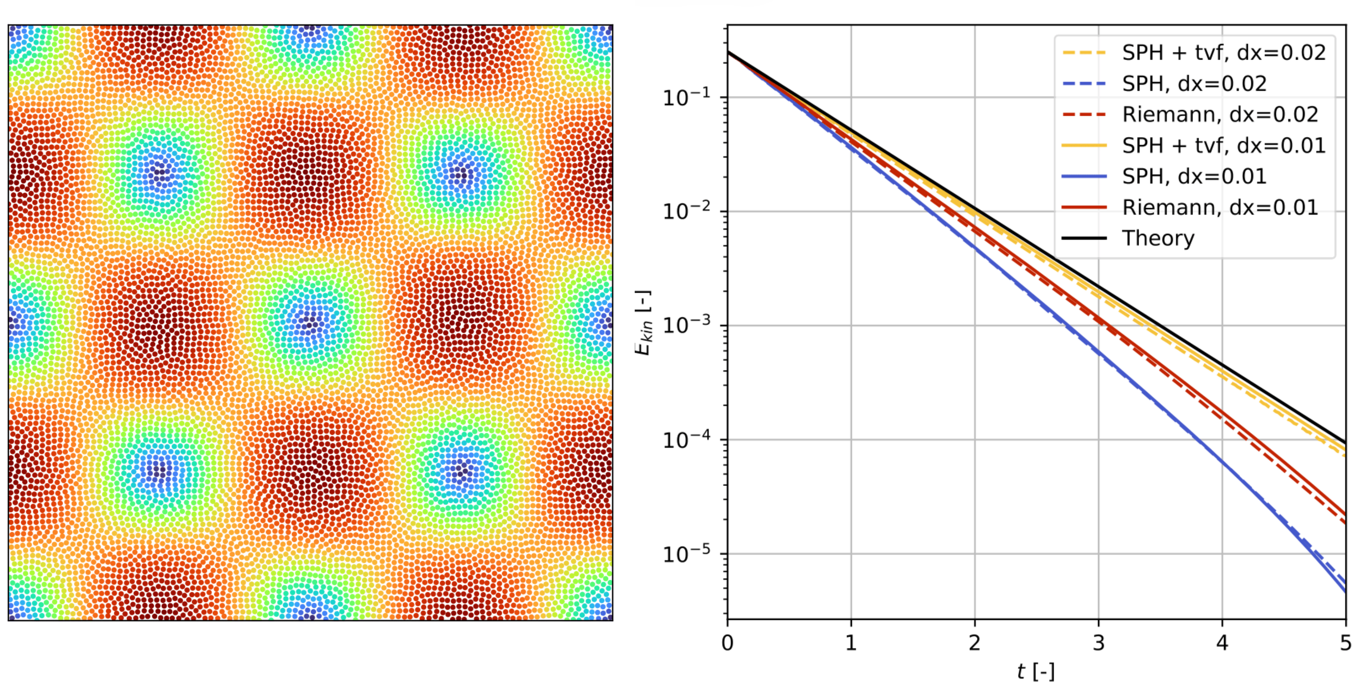
We introduce the first JAX-based weakly compressible SPH solver for simulating incompressible fluids. The governing equations of such systems are the mass and momentum conservation equations

$$\frac{d}{dt}(\rho) = -\rho(\nabla \cdot \mathbf{u}),$$
$$\frac{d}{dt}(\mathbf{u}) = -\frac{1}{\rho}\nabla p + \frac{1}{Re}\nabla^2 \mathbf{u} + f_{ext},$$

where ρ denotes the density, $\mathbf{u}$ the velocity, p the pressure, Re the Reynolds number, and $\mathbf{f}$ the external force. Our SPH framework includes the following components:

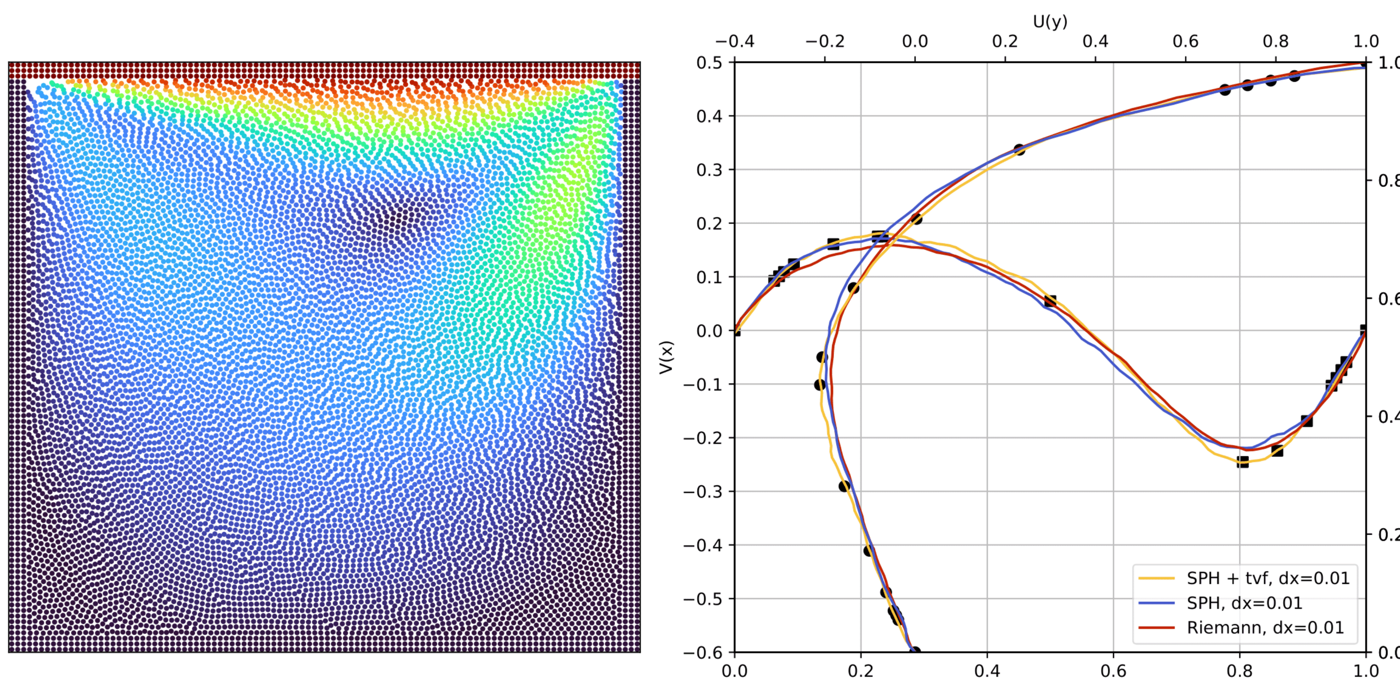
- Standard SPH - weakly compressible SPH solver, see [Adami et al., 2012]
- Transport velocity formulation SPH - improved shifting scheme, see [Adami et al., 2013]
- Riemann SPH - low-dissipation SPH solver solving 1D Riemann problems between the particles, see [Zhang et al., 2017]
- Wall boundary condition (BC) - *free-slip* and *no-slip* boundary conditions, see [Adami et al., 2012]
- Thermal diffusion - diffusive temperature field with Dirichlet BC

2D Taylor Green Vortex



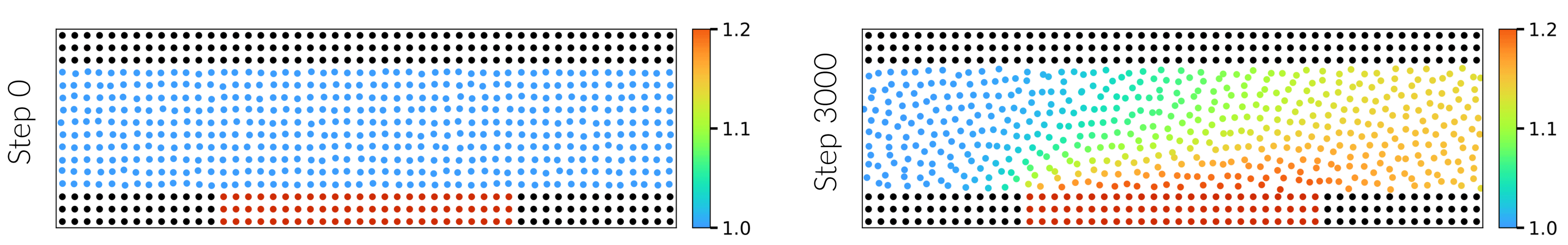
2D Taylor Green vortex velocity magnitudes at the start of the simulation (left) and at $t = 5$ (right), calculated using transport velocity formulation SPH.

2D Lid-Driven Cavity



Lid-driven cavity with $dx = 0.01$ showing absolute particle velocities of the Riemann solver (left) and velocity profiles of each SPH method at the midsection for U and V (right)

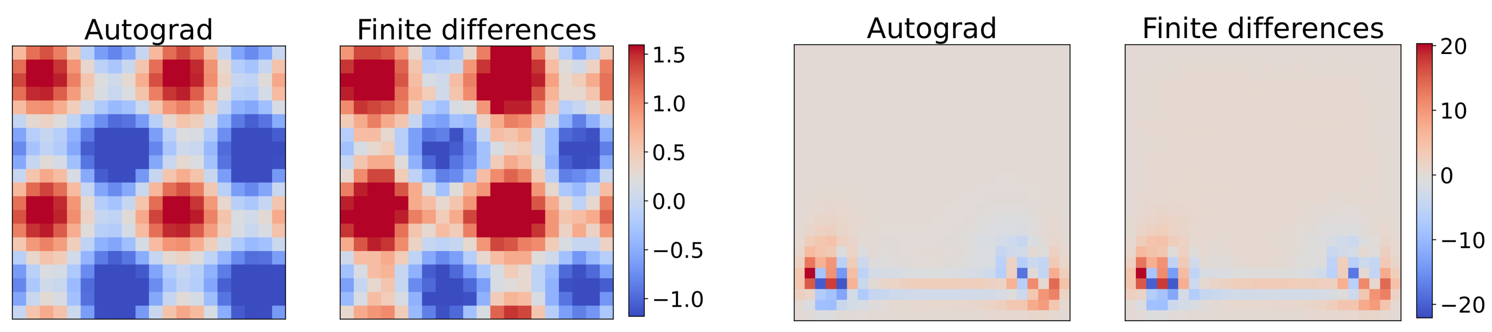
Thermal Diffusion Example



Simulation of channel flow with hot bottom wall using standard SPH and thermal diffusion. The plots show the non-dimensional temperature at different time steps.

Gradient Validation

Solver gradients of kinetic energy over position changes $\frac{dE_{kin}}{dr}$, comparing JAX Autograd to finite differences on Taylor-Green vortex and lid-driven cavity.

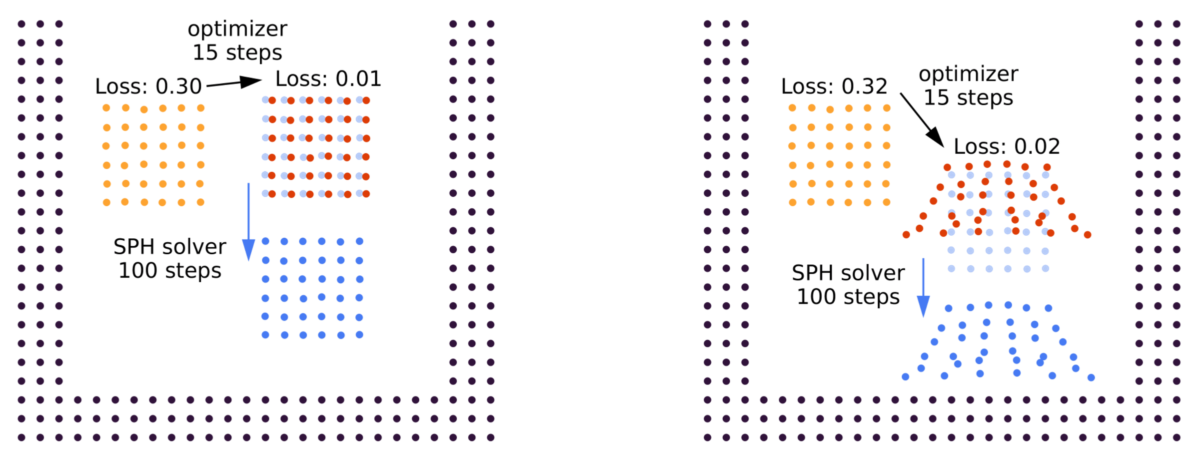


Taylor-Green Vortex   Lid Driven Cavity

Machine Learning Applications

Inverse Problem

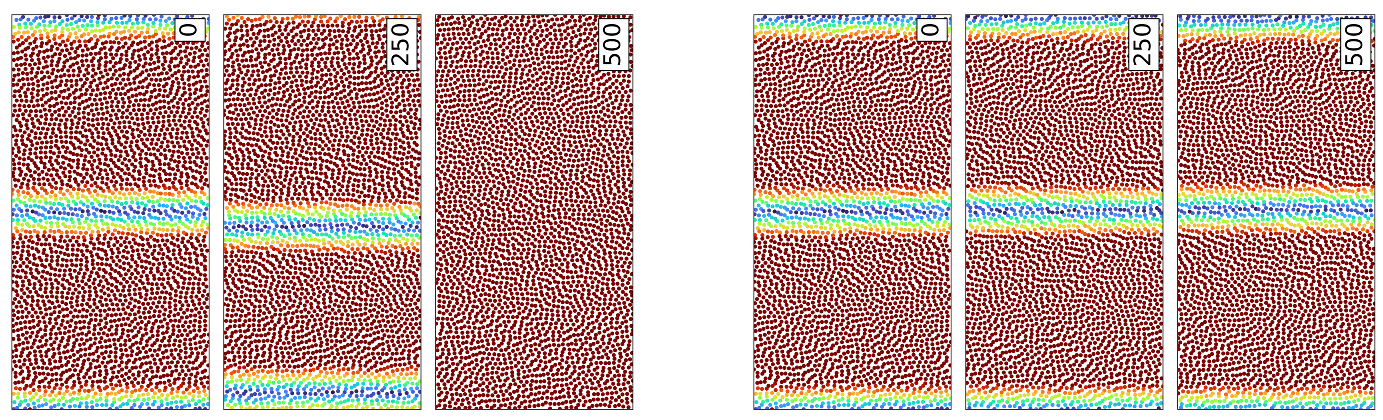
- A 2D water cube inside a box undergoes acceleration due to gravity.
- The task is to find the initial position of the cube given its final state.
- MSE between the target final state and the simulated final state with random initial particles is used as loss to optimize the positions.



Solver-in-the-Loop

- We adapt the popular *"Solver-in-the-Loop"* (SitL) [Um et al., 2021] training scheme to particles.
- SitL interleaves a traditional solver a coarse spatial and/or temporal discretization with a learnable correction function.
- The solver needs to be differentiable, as gradients are computed through it for multiple rollout steps in training.

Metric	Solver only	Learned only	SitL
MSE_5	$1.7e-7$	$6.7e-9$	$\mathbf{3.3e-9}$
MSE_{20}	$7.9e-6$	$1.9e-7$	$\mathbf{1.3e-7}$
$MSE_{E_{kin}}$	0.13	$2.8e-4$	$\mathbf{7.4e-5}$
Sinkhorn	$3.4e-7$	$3.7e-8$	$\mathbf{9.3e-9}$



Learned only (single step)   SitL (3 steps)

References

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