Fully Lagrangian Approach in OpenFOAM: implementation and preliminary results

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Vortex rings and related problems
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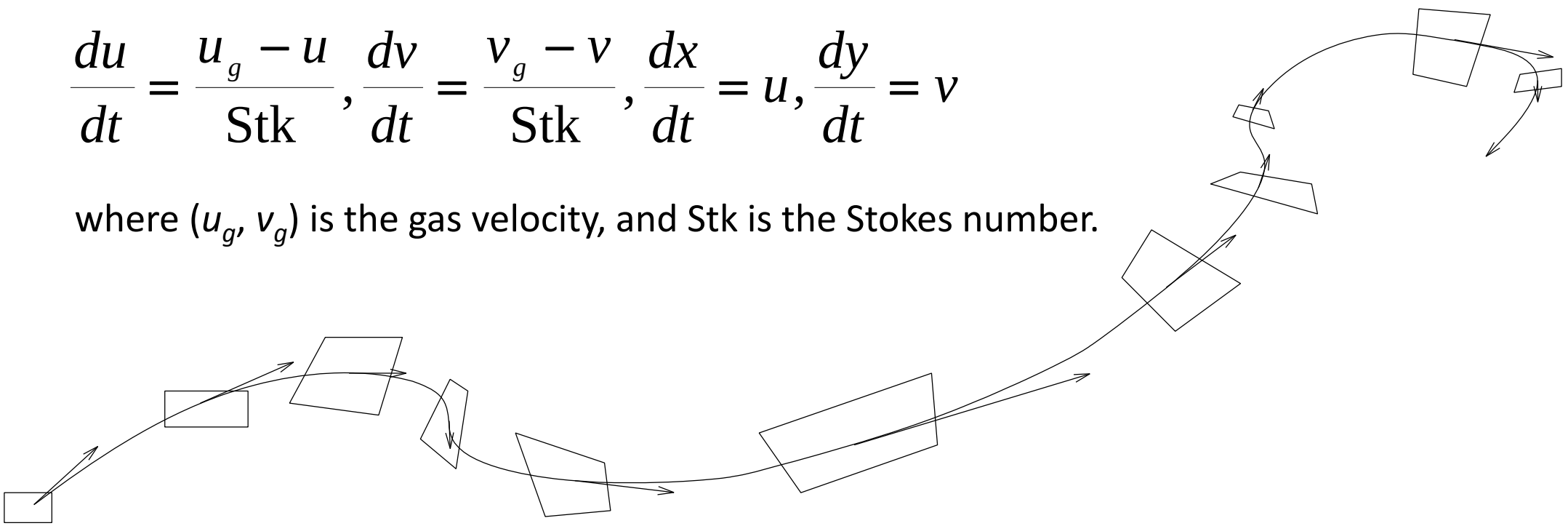
Overview

- Fully Lagrangian approach (FLA)
- FLA in ANSYS Fluent and why OpenFOAM?
- Overview of FLA implementation into OpenFOAM Lagrangian subsystem
- Test case: number density of particles in a flow around cylinder

Fully Lagrangian approach (FLA)

$$\frac{du}{dt} = \frac{u_g - u}{\mathrm{Stk}}, \frac{dv}{dt} = \frac{v_g - v}{\mathrm{Stk}}, \frac{dx}{dt} = u, \frac{dy}{dt} = v$$

where (u_g, v_g) is the gas velocity, and Stk is the Stokes number.



$$n(x_0, y_0, t) = \det\|J\| n(x_0, y_0, 0)$$

Fully Lagrangian approach (FLA)

$$J_{11} = \frac{\partial x}{\partial x_0}, J_{12} = \frac{\partial x}{\partial y_0}, J_{21} = \frac{\partial y}{\partial x_0}, J_{22} = \frac{\partial y}{\partial y_0}$$

$$\frac{dJ_{11}}{dt} = w_{11}, \frac{dJ_{12}}{dt} = w_{12}, \frac{dJ_{21}}{dt} = w_{21}, \frac{dJ_{22}}{dt} = w_{22}$$

$$\frac{dw_{11}}{dt} = \frac{1}{\mathrm{Stk}}\left(J_{11}\frac{\partial u_g}{\partial x} + J_{21}\frac{\partial u_g}{\partial y} - w_{11} \right), \quad \frac{dw_{12}}{dt} = \frac{1}{\mathrm{Stk}}\left(J_{12}\frac{\partial u_g}{\partial x} + J_{22}\frac{\partial u_g}{\partial y} - w_{12} \right), \qquad (1)$$

$$\frac{dw_{21}}{dt} = \frac{1}{\mathrm{Stk}}\left(J_{11}\frac{\partial v_g}{\partial x} + J_{21}\frac{\partial v_g}{\partial y} - w_{21} \right), \quad \frac{dw_{22}}{dt} = \frac{1}{\mathrm{Stk}}\left(J_{12}\frac{\partial v_g}{\partial x} + J_{22}\frac{\partial v_g}{\partial y} - w_{22} \right).$$

FLA in ANSYS Fluent CFD

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A model for heating and evaporation of a droplet cloud and its implementation into ANSYS Fluent

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Atomization and Sprays, 27(6): 493–510 (2017)

FLA implemented as dll extension using User Defined Functions

THE FULLY LAGRANGIAN APPROACH TO THE ANALYSIS OF PARTICLE/DROPLET DYNAMICS: IMPLEMENTATION INTO ANSYS FLUENT AND APPLICATION TO GASOLINE SPRAYS

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Why not ANSYS Fluent?

- Low control and flexibility (closed source)
- Two-way coupling is tricky
- Poor reproducibility (manual case setup in GUI, can’t easily compare parameters of cases)

Why OpenFOAM?

- Full control (Open Source)
- Great reproducibility (case setting are defined in plaintext files)

FLA in OpenFOAM: implementation strategy for steady-state two-way coupled solver

- **Case** level:
  - Let user choose initial conditions for $\boldsymbol{J}$ and $\boldsymbol{w}$ (Omega)
  - Handle IO (saving results, restarting calculations)
  - Integrate with existing postprocessing tools (ParaFoam)
- **Solver** level (high level combination of existing building blocks):
  - Iterate between calculations for carrier and dispersed phases
  - Calculate **grad(U)** and pass it to Lagrangian particle tracker
- **Lagrangian library** level (building block):
  - Add $\boldsymbol{J}$ and $\boldsymbol{w}$ (Omega) as particle properties
  - Integrate $\boldsymbol{J}$ and $\boldsymbol{w}$ (Omega) along the particle trajectory
  - Update appropriate source terms in the cell containing the particle

Solver level: modify existing SIMPLE solver

```
basicKinematicCloud\
    parcels("kinematicCloud", rhoInf, U, mu, GradU, g);
while (simple.loop(runTime))
{
    parcels.evolve();

    // --- Pressure-velocity SIMPLE corrector
    {
        #include "UEqn.H"
        #include "pEqn.H"
    }
    // @tz need this for FLA, is used by parcels
    GradU = fvc::grad(U);

    laminarTransport.correct();
    turbulence->correct();
    runTime.write();
}
```

Lagrangian library level

- **Cloud** is a collection of parcels with different physical properties.
- **Parcel** is a collection of particles with the same physical properties.
- **Particle** is responsible for tracking position in the mesh.

Actual physics is in the parcel.

Relevant files are located at:
OpenFOAM/src/lagrangian/intermediate/parcels/Templates/KinematicParcel/

KinematicParcel.H: J, Omega

```
class KinematicParcel
{
    // @tz components of the
    Jacobian and auxilary variables
    tensor J_;
    tensor Omega_;

    inline const tensor& J() const;
    inline const tensor& Omega()
    const;
    inline tensor& J();
    inline tensor& Omega();
}
```

Access to carrier phase properties in the cell:

```
class trackingData
{
    // @tz We need the continuous phase
    velocity gradient in the cell
    tensor GradUc_;
    inline const interpolation<tensor>&
    GradUInterp() const;
    inline const tensor& GradUc()
    const;
    inline tensor& GradUc();
}
```

KinematicParcel.C: KinematicParcel::calc

```
void Foam::KinematicParcel<ParcelType>::calc
{
    // Linearised momentum source coefficient
    scalar Spu = 0.0;
    this->U_ = calcVelocity(cloud, td, dt, Re, td.muc(), mass0, Su,
    dUTrans, Spu);

    this->Omega_.xx() = this->Omega_.xx() + Spu*(
            this->J_.xx()*td.GradUc().xx()
            + this->J_.yx()*td.GradUc().xy()
             - this->Omega_.xx());
    // repeat for all components of Omega

    this->J_ = this->J_ + this->Omega_*dt;
    // Accumulate carrier phase source terms
    // {…}
}
```

KinematicParcel.C: KinematicParcel::calc

```
// Accumulate carrier phase source terms
// ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
if (cloud.solution().coupled())
{
    scalar n_d = 1./ fabs(det(this->J_));

    // Update momentum transfer
    cloud.UTrans()[this->cell()] += n_d*np0*dUTrans;

    // Update momentum transfer coefficient
    cloud.UCoeff()[this->cell()] += n_d*np0*Spu;
}
```

KinematicParcel: Constructors + IO

- **KinematicParcelI.H**
  Modify all constructors to account for J, Omega
  Implement access functions for J, Omega

- **KinematicParcelIO.H**
  Modify all input-output functions to account for J, Omega

- **KinematicParcelTrackingDataI.H**
  Modify constructor to account for GradUInterp and GradUc
  Implement access functions for GradUInterp and GradUc

FLA injection model: J0, Omega0

Located at:
lagrangian/intermediate/submodels/Kinematic/InjectionModel/PatchInjection/

PatchInjection.H

```
class PatchInjection
{
    //- @tz
    const tensor J0_;
    const tensor Omega0_;
}
```

PatchInjection.C

```
Foam::PatchInjection<CloudType>::PatchInjection
:
    J0_(this->coeffDict().lookup("J0")),
    Omega0_(this->coeffDict().lookup("Omega0"))

void
Foam::PatchInjection<CloudType>::setProperties
{
    parcel.J() = J0_;
    parcel.Omega() = Omega0_;
}
```

What does this give us?

- Two-way coupled steady state solver for kinematic particles in fluid flow
- OpenFOAM takes care of under-relaxation of fluid flow equations (don't have to worry about source terms being too big)
- Library code can be reused as it is to build transient solvers
- Integration with OpenFOAM case structure (no hardcoded parameters that require recompilation to change)
- Integration with ParaFoam (postprocessing)

Ongoing work

- Validation and verification
- Equations for Omega can be rewritten in more general tensor form
- More general approach to setting J/Omega integration schemes (currently there is only hardcoded Euler scheme)

Flow around cylinder

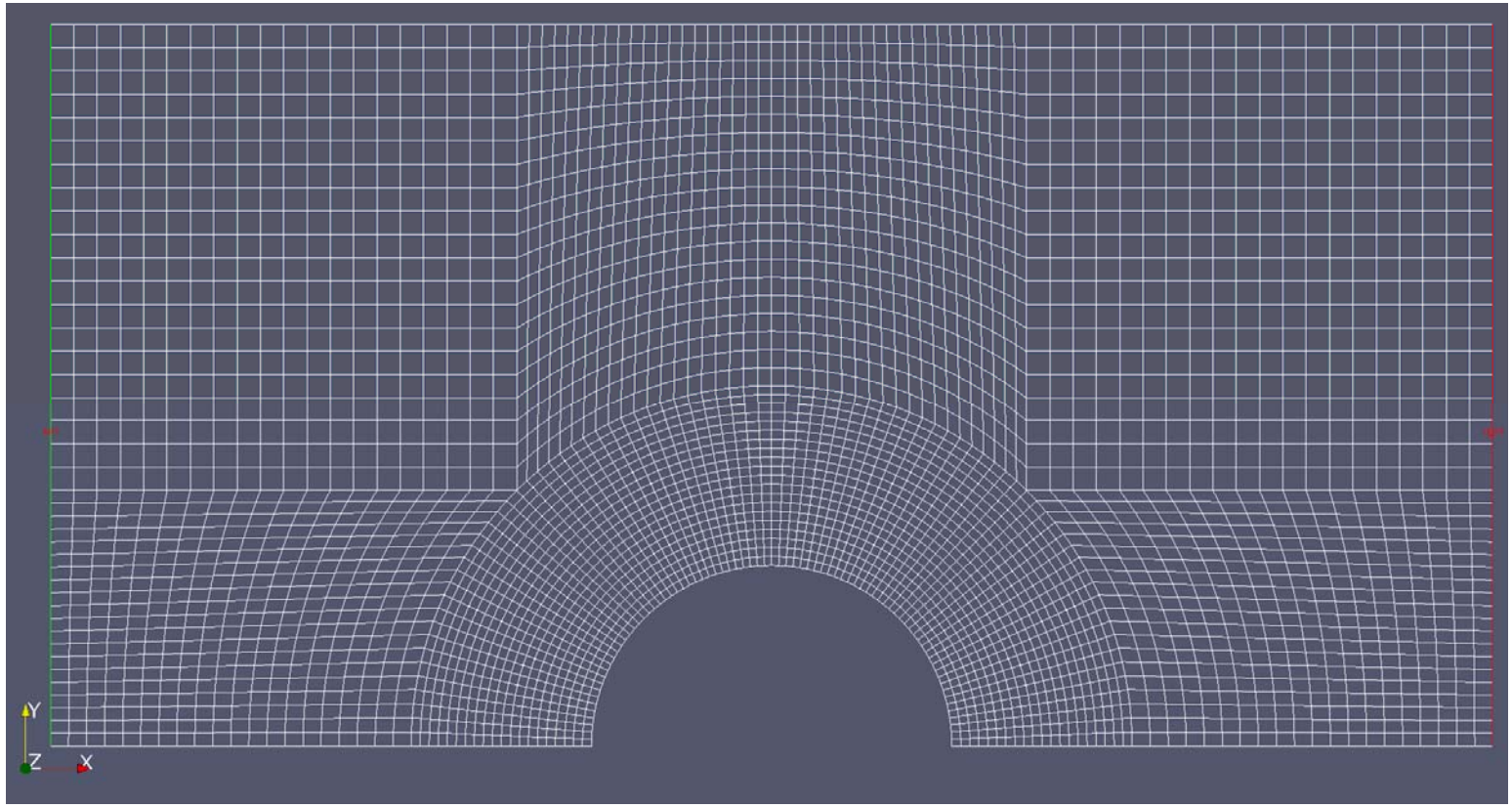
Cylinder radius:
R = 0.05 m

Domain height 0.2 m
Domain width 0.4 m

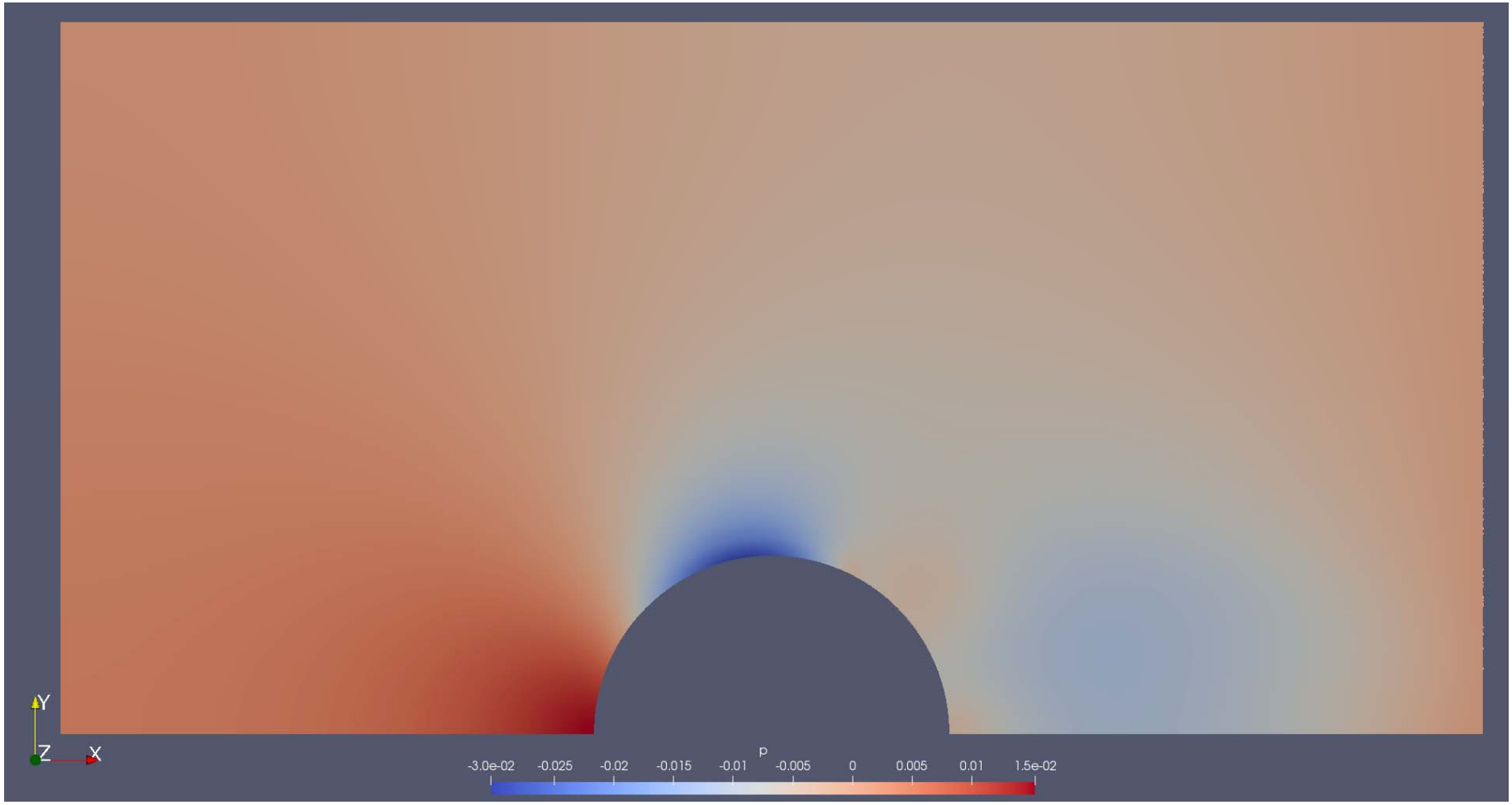
left (green):
U0 = 0.15 m/s

right (red):
P = 0

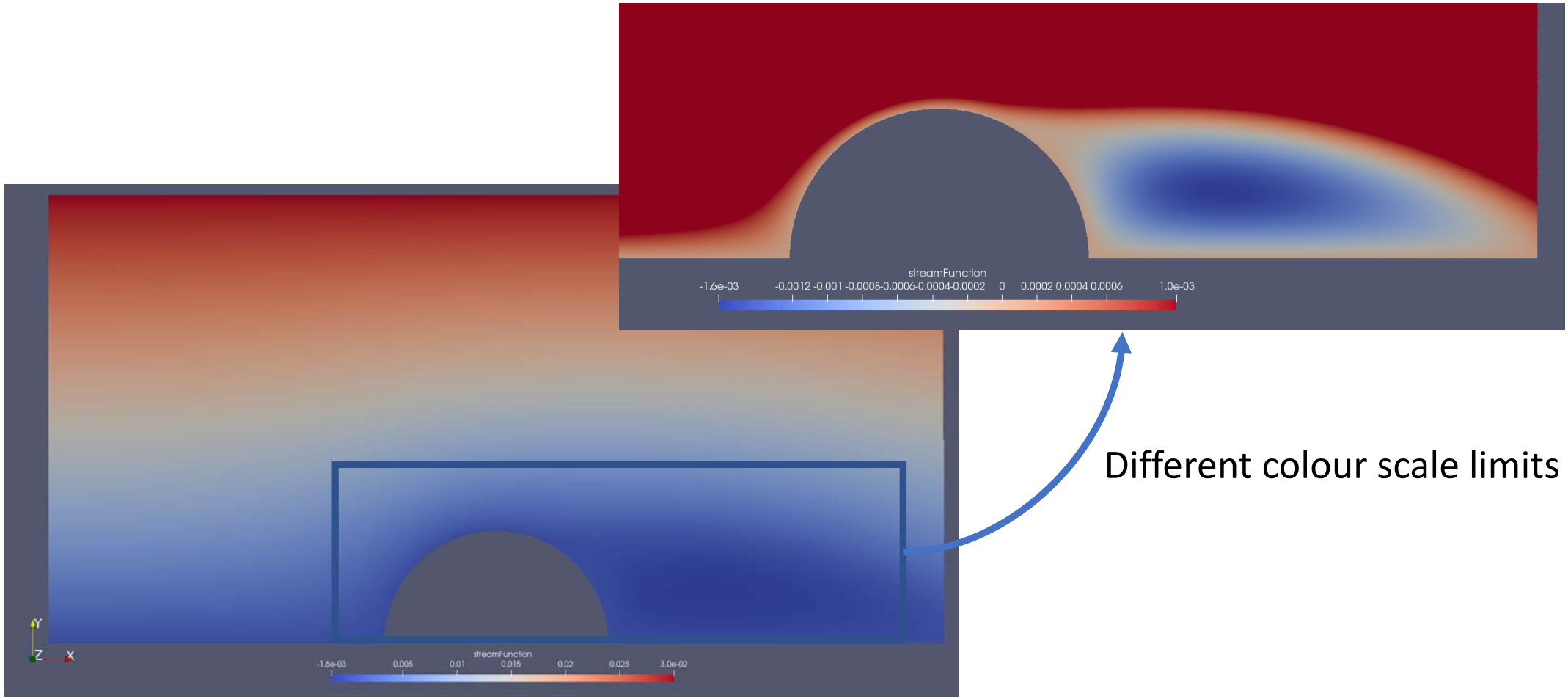
Symmetry at all other boundaries.



Pressure contour



Stream function contour



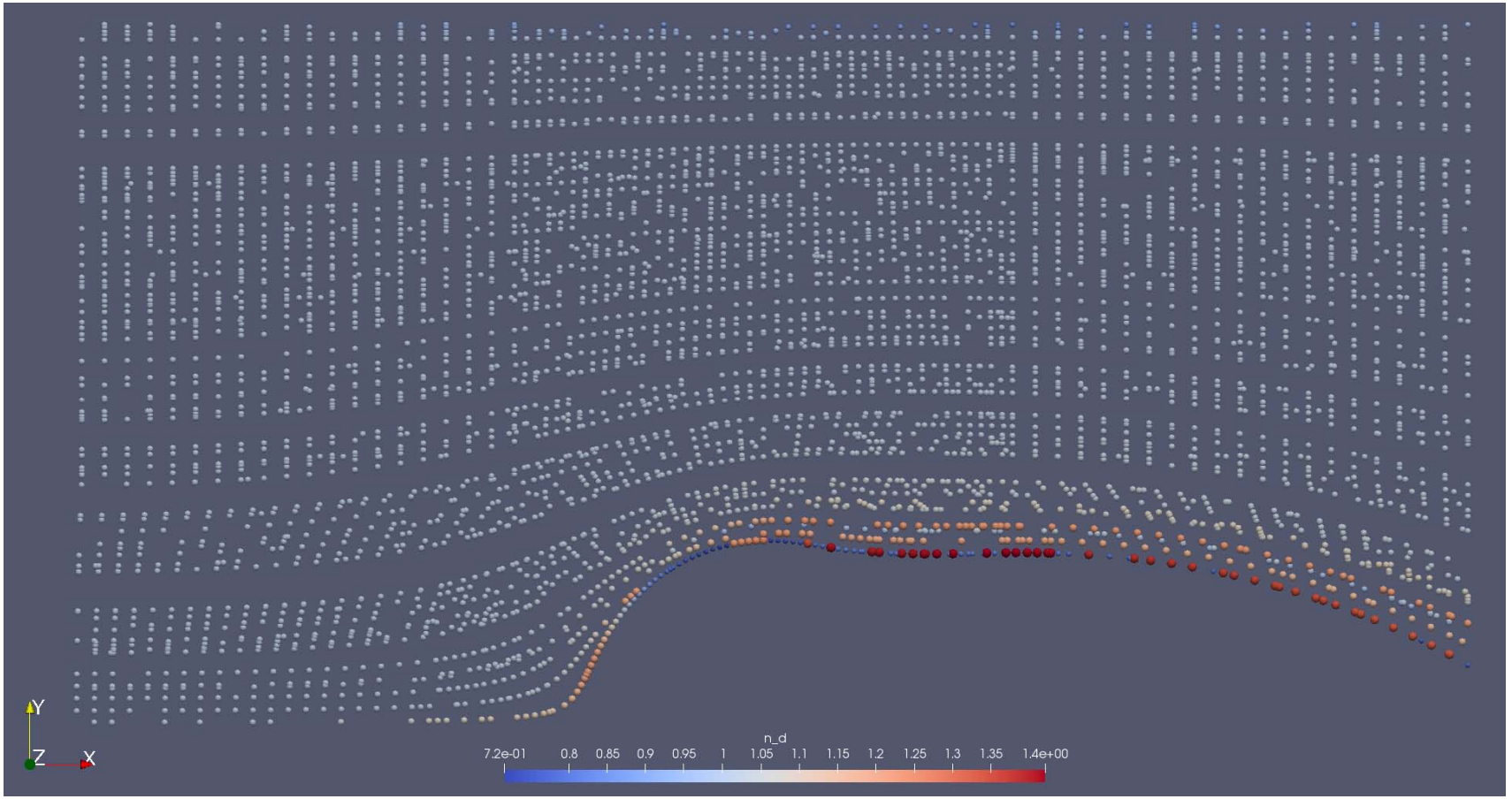
Different colour scale limits

Particle trajectories coloured by number density

Starting at the left boundary with
V0 = 0.15 m/s

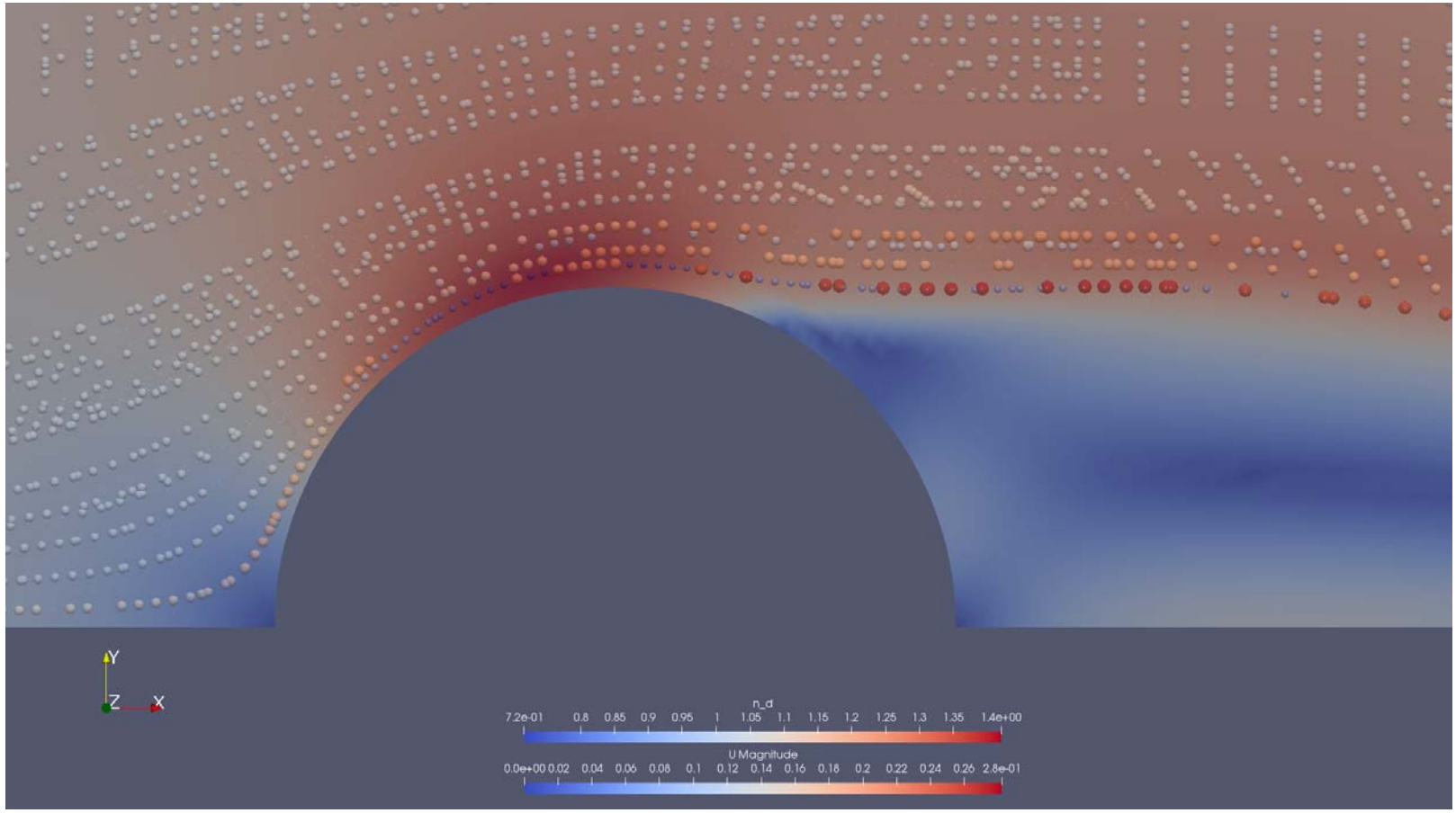
Material: water

Diameter: 5e-5 m



Particle trajectories on top of flow velocity magnitude contour

Number density represented by size and colour of the spheres



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Thank you!