

Rayleigh-Bénard Convection: Drekar Simulation on Odyssey

Harvard IACS AC 290R

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Problem Statement & Motivation

- Rayleigh-Bénard Convection (RBC) arises when a fluid has a temperature gradient in a gravitational field
 - It is an important physical phenomenon arising in stellar evolution, plate tectonics, and weather systems
- We ran a numerical simulation of RBC based on the Boussinesq approximation
- The simulation was run on Odyssey using the Drekar code developed at Sandia National Lab

Description of Code

- Drekar is a large scale computational fluid dynamics (CFD) code developed at Sandia National Lab
- Drekar solves fluid PDEs using the Finite Element Method (FEM)
- Core functionality is a massively parallel FEM implementation that runs on MPI, as well as OpenMP and CUDA
- Drekar is part of the Trilinos suite of packages, which provides functionality including linear algebra, nonlinear solvers, automatic differentiation, and time integration

Software Behind The Simulation

- Initially, **ParaView** locally to prototype
- **Batch** job
 - **SLURM** for job management
- **XML** description file
 - Could have used **YAML**
- **Pamgen** to define the finite element grid
 - Alternatives for mesh definition exist
- **Exodus** for storing and accessing finite element analysis
 - **epu** to merge it all

Refactoring

```
ac290ru1904@boslogin02:/n/scratchlfs/ac290r/project1
```

```
$ tree -L 2
```

```
.
├── case1024
│   ├── case1024.err
│   ├── case1024.out
│   ├── case1024.pam
│   ├── case1024.sh
│   ├── case1024.xml
│   ├── drekar.exe -> /n/home02/ac290ru1904/SoftwareLibraries/drekar-gcc-RELEASE/DrekarBase/drekar/bin/drekar.exe
│   ├── exo
│   └── rename.sh
└── case512
    ├── case512.err
    ├── case512.out
    ├── case512.pam
    ├── case512.sh
    ├── case512.xml
    ├── drekar.exe -> /n/home02/ac290ru1904/SoftwareLibraries/drekar-gcc-RELEASE/DrekarBase/drekar/bin/drekar.exe
    ├── exo
    └── rename.sh
```

Overview of Numerical Methods Used

- The Finite Element Method (FEM) solves PDEs by discretizing them in space on a *mesh*.
- The functions to be solved for (here pressure, temperature, and velocity) are represented by choosing a finite dimensional basis
- This simulation used piecewise polynomials of order 1, i.e. rectilinear planar functions (analog to piecewise linear in 2D)
- The time stepper discretizes in time; each time step leads to a set of linear equations to be solved and then a nonlinear solution

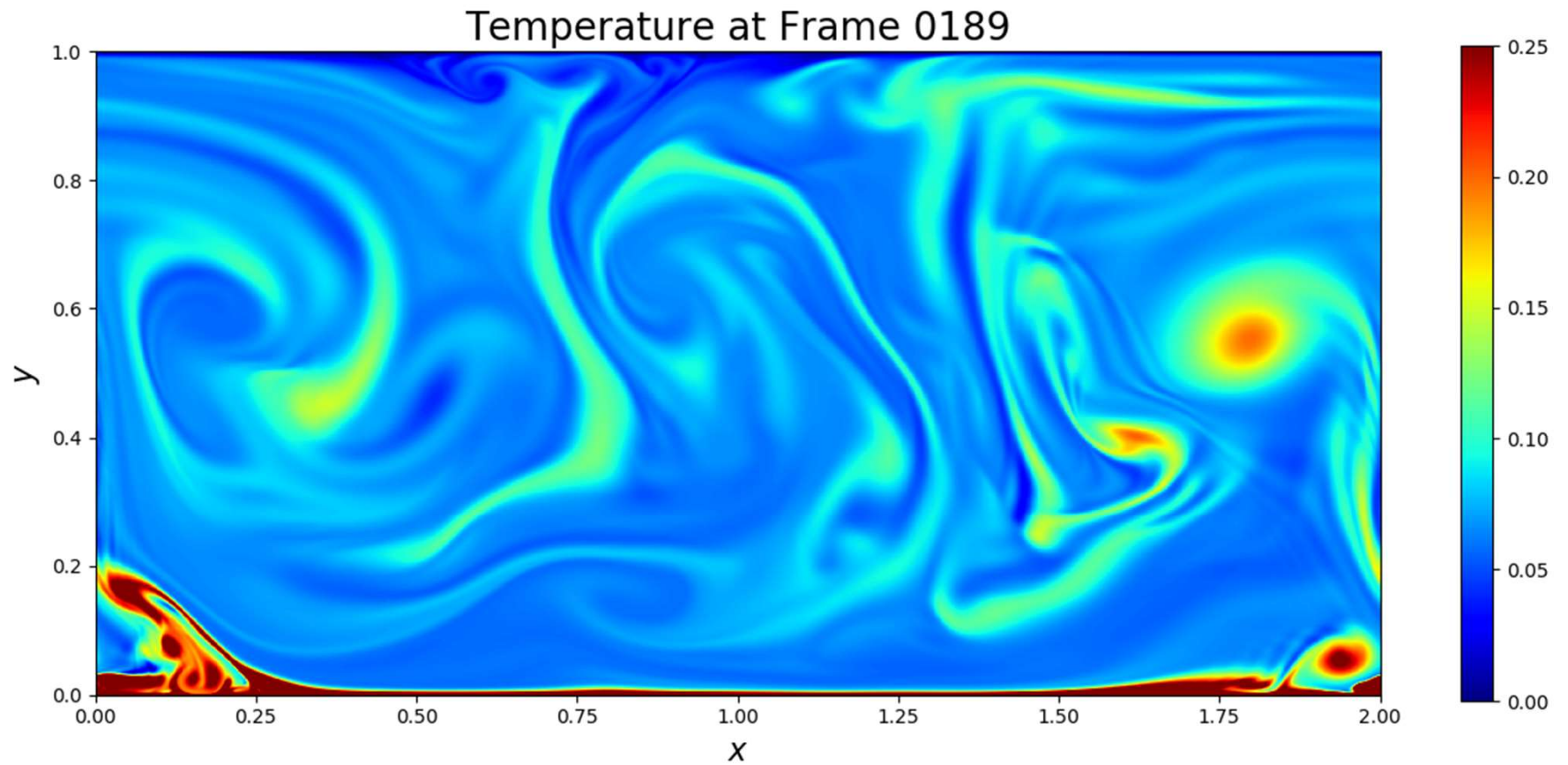
Parameters of the Simulation

- Dimensions: Length $L=2.0$, Height $=1.0$, $\Gamma = 2$; $N_x = 2048$, $N_y = 1024$
- Density $\rho_0 = 1.0$
- Viscosity $\nu = 0.01$
- Volume Expansion Coefficient $\alpha_v = 10^6$
- Gravity $g = 1.0$
- Heat Capacity $C_p = 1.0$
- Thermal Conductivity $k = 0.01$
- Thermal diffusivity $\kappa = k / \rho_0 C_p = 0.01$
- Temperature Change $\Delta T = 1.0$; time dependent $\Delta T = 1 - \exp(-t/0.2)$
- Time of Simulation: 5.0 target (0.22 achieved on case 1)

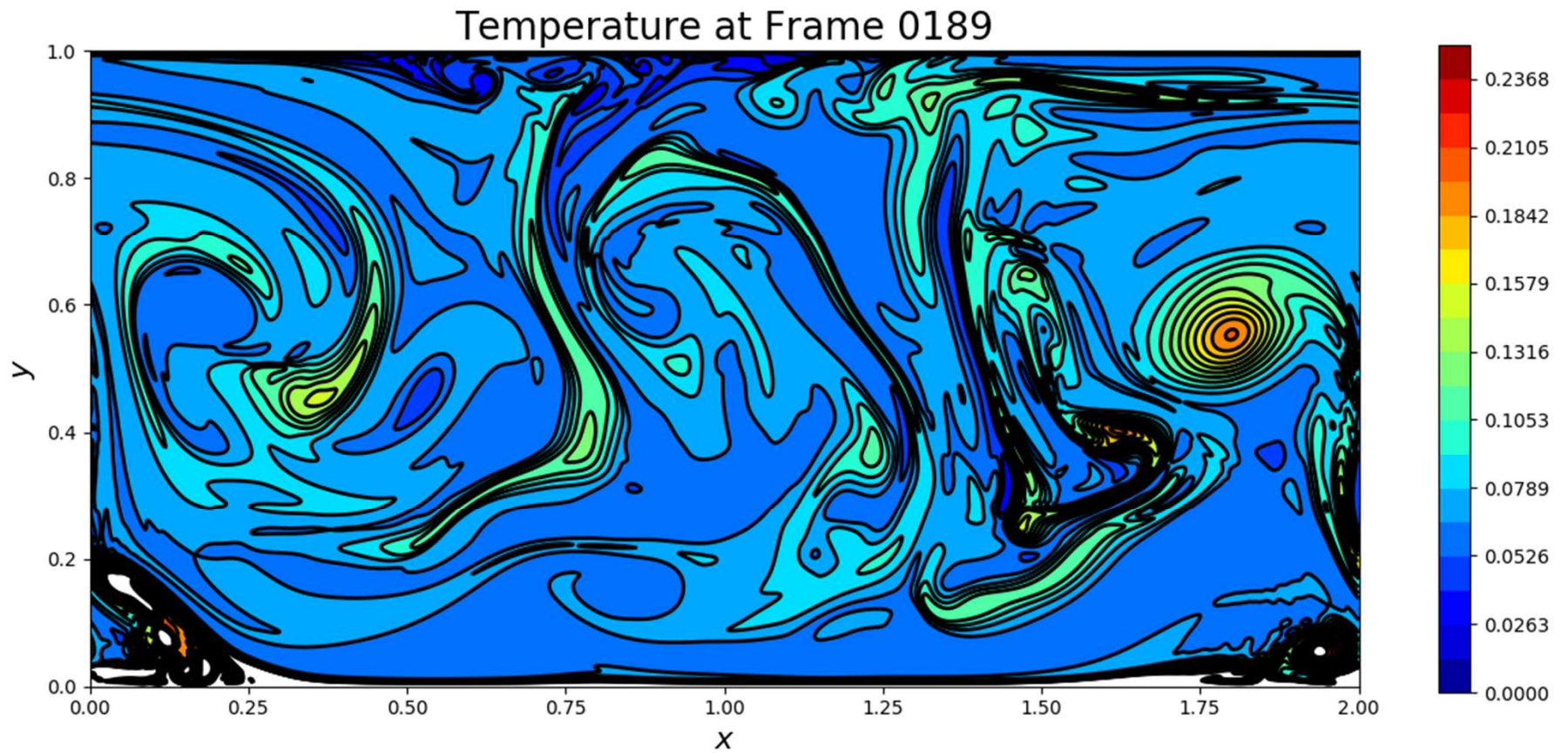
Results

- Case 1 was initiated on 1024 cores but only ran on 512 cores due to a hardware fault.
- It ran for about 1 day and got to time 0.22 before we restarted it.
- Case 2 ran on all 1024 cores for about 5 days. It bogged down, getting progressively slower, and eventually crashed (out of memory)
- It only got to a simulation time of 0.77; it should have gotten much further. After it crashed, our .exo output files became corrupted.
- We suspect a memory leak
- We present visualizations from the successful case 1 simulation

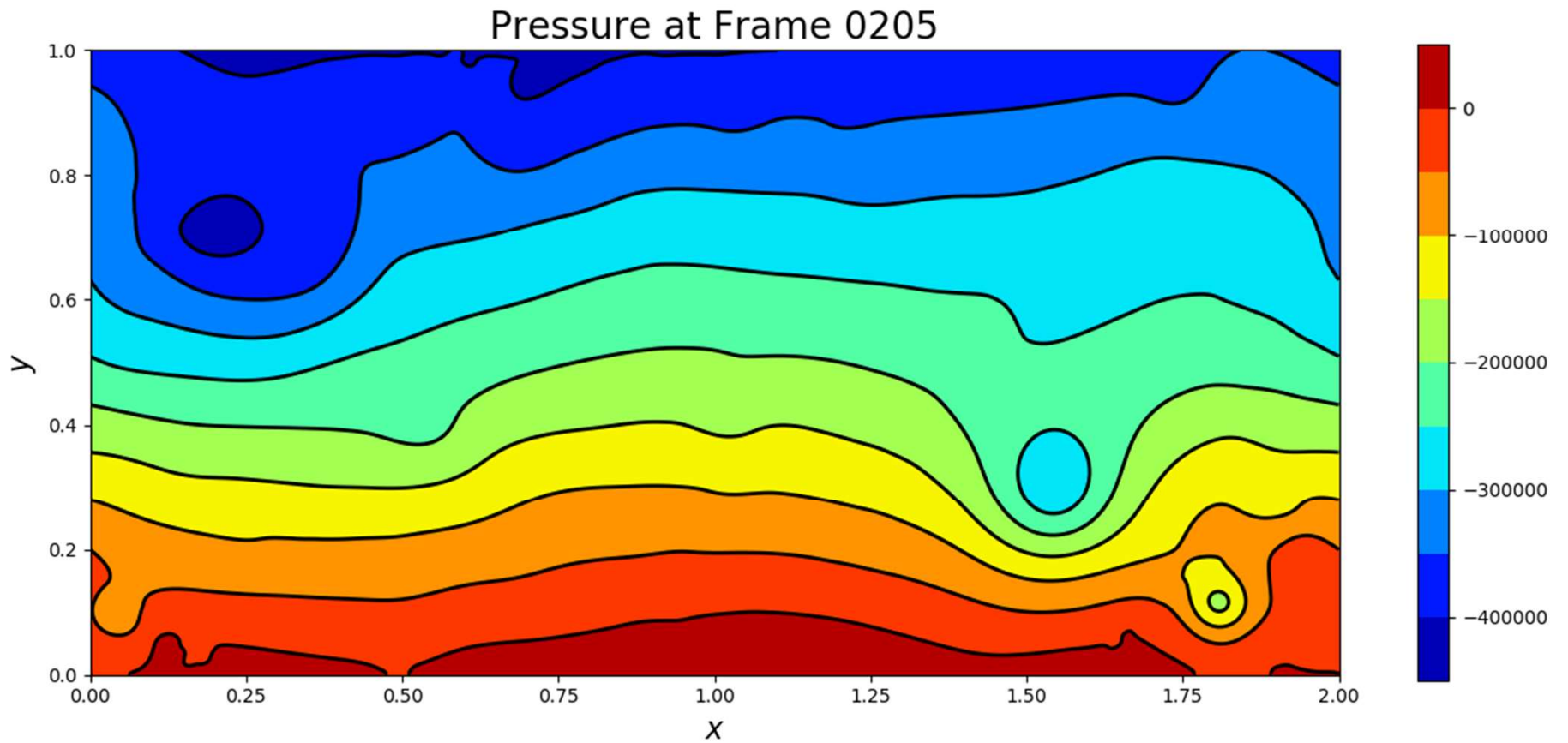
Sample Output: Temperature



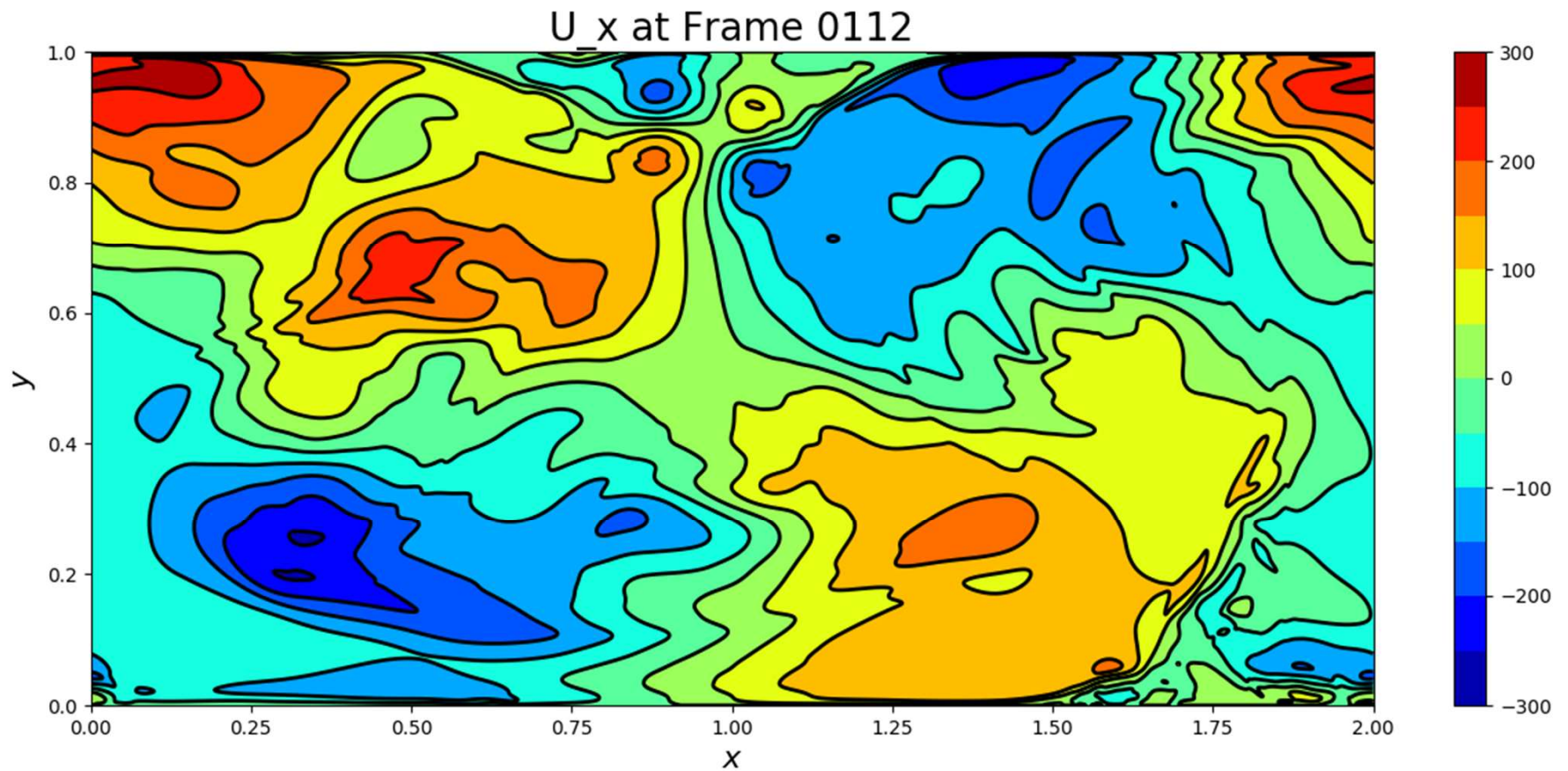
Sample Output: Temperature



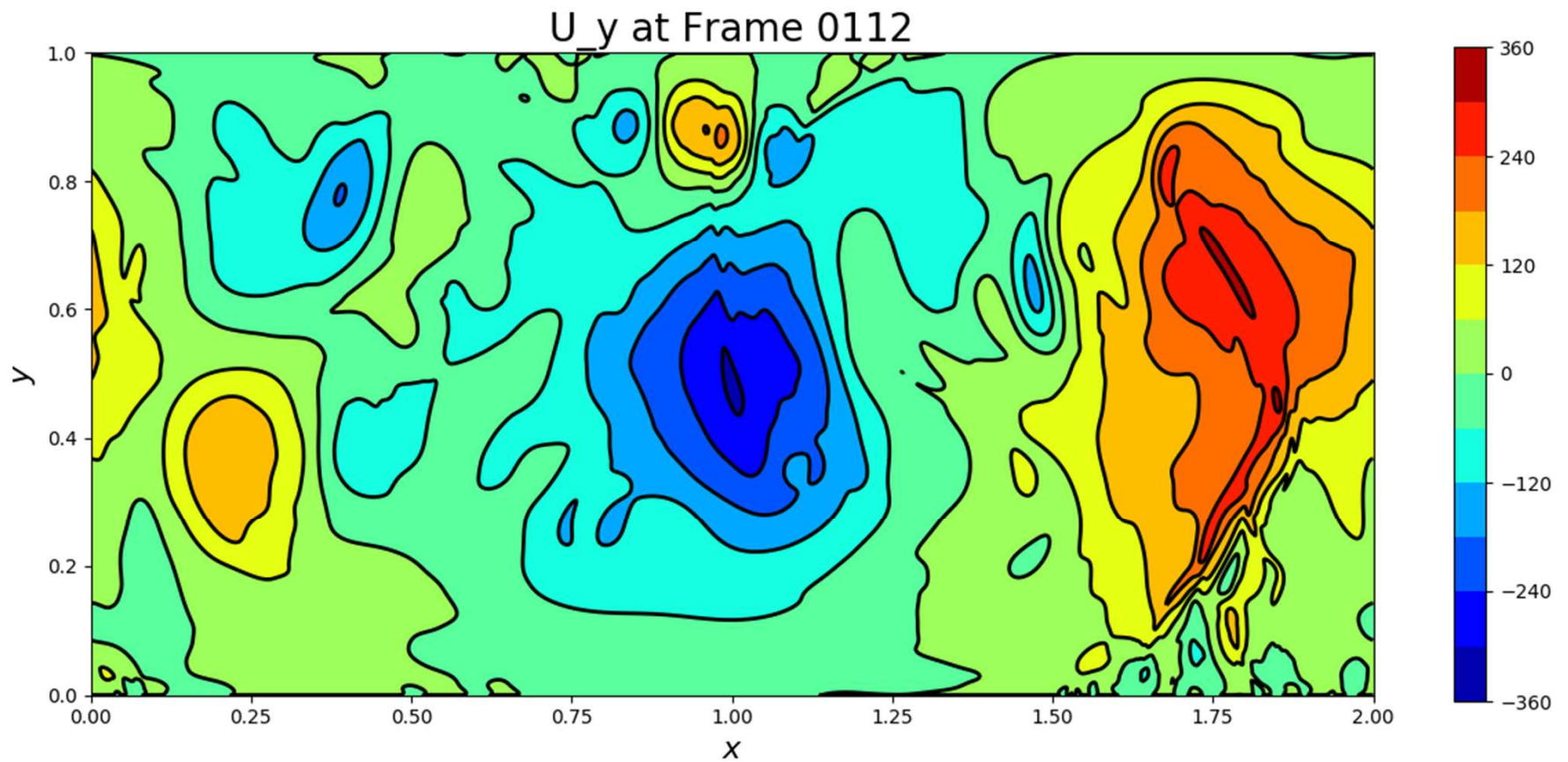
Sample Output: Pressure



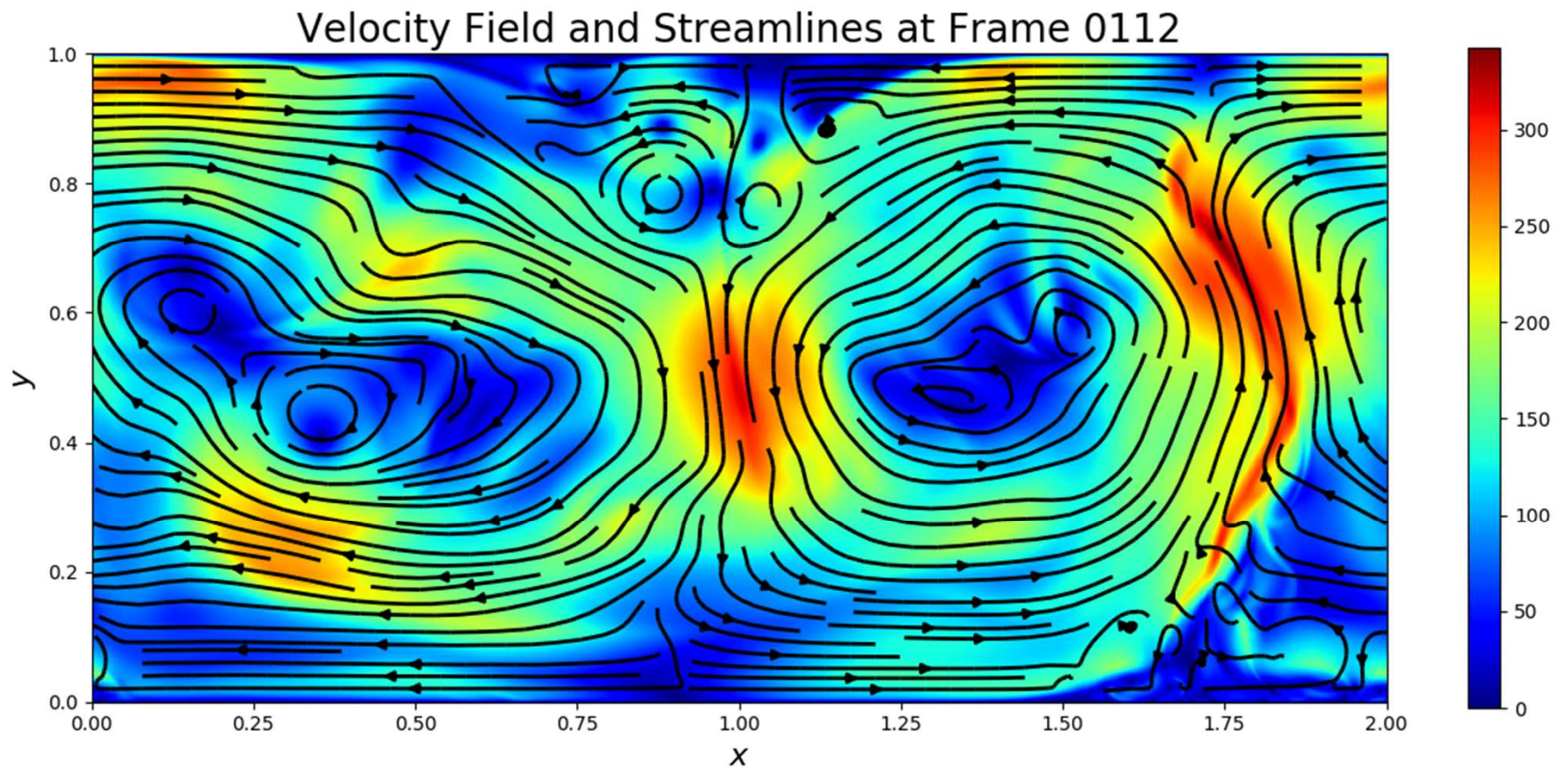
Sample Output: Velocity in x Direction



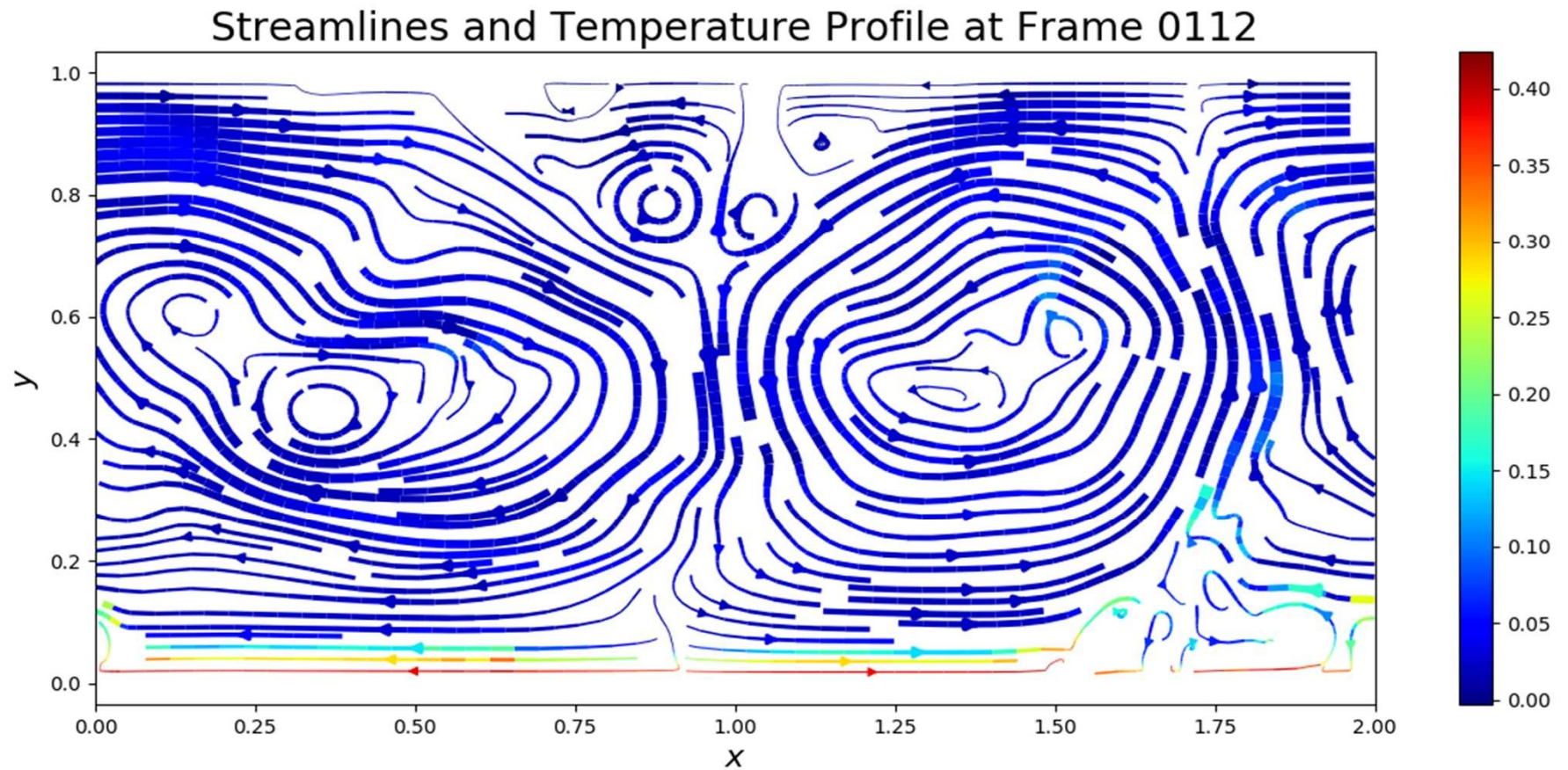
Sample Output: Velocity in y Direction



Sample Output: Velocity & Streamlines

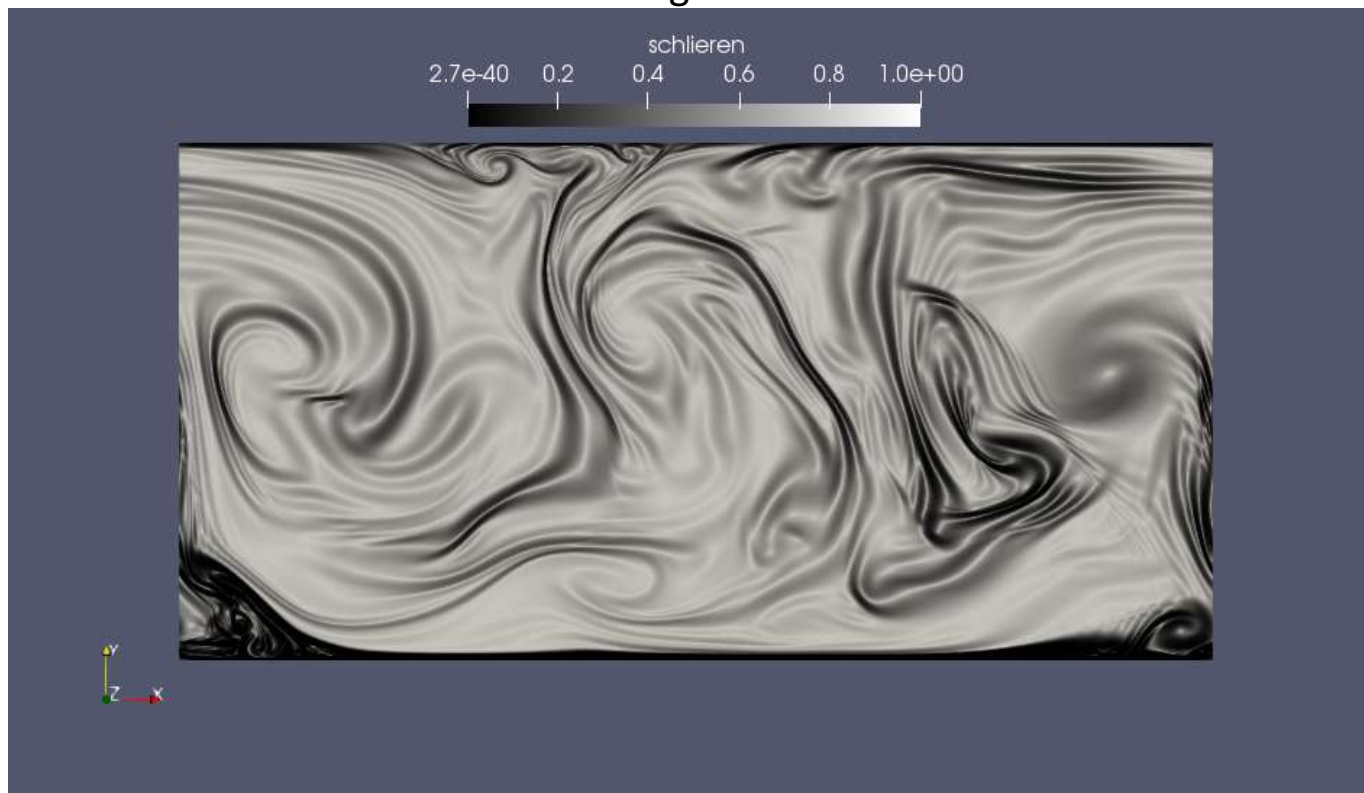


Sample Output: Streamlines & Temperature



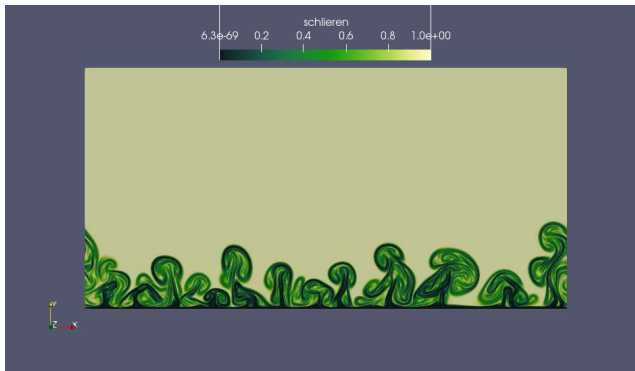
Sample Output: Schlieren Flow Visualization

Schlieren Image at Frame 190

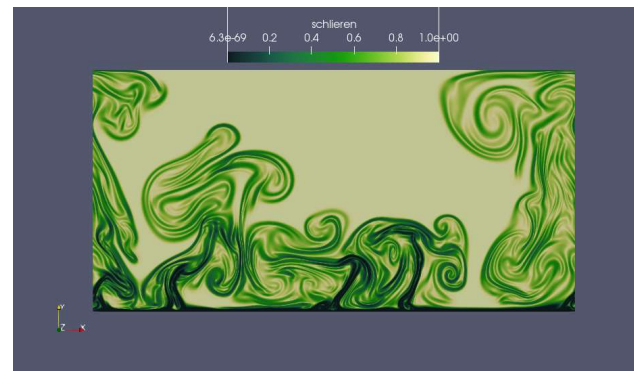


Sample Output: Schlieren Flow Visualization

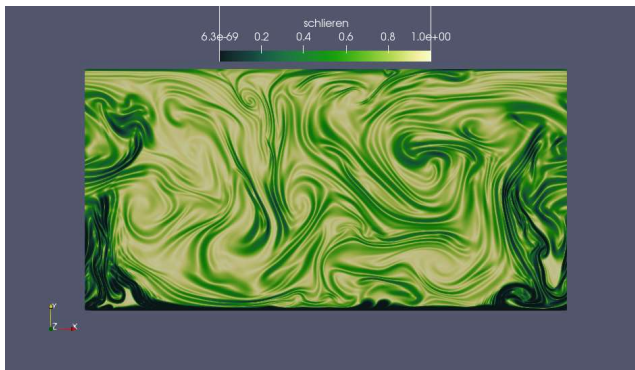
Schlieren Image at Frame 044



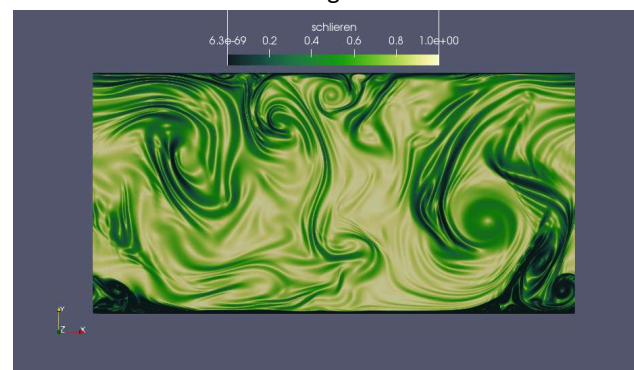
Schlieren Image at Frame 062



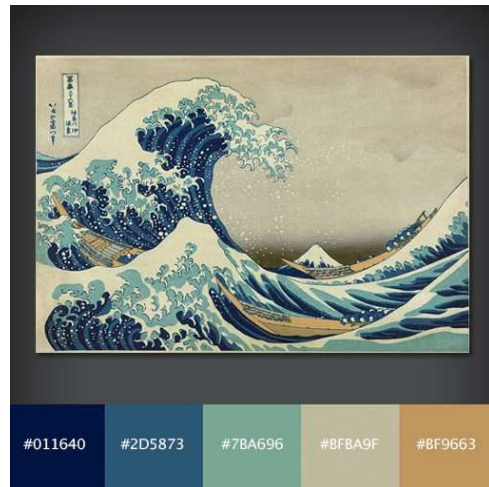
Schlieren Image at Frame 102



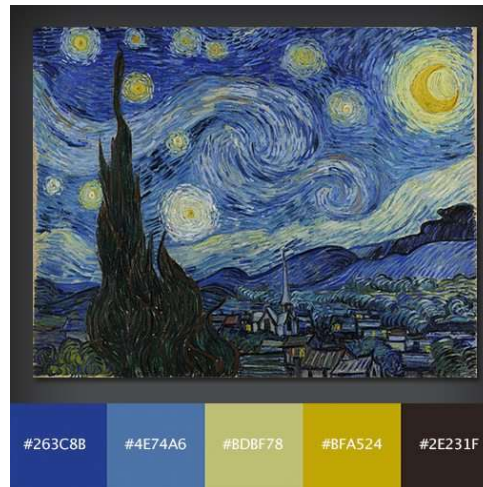
Schlieren Image at Frame 206



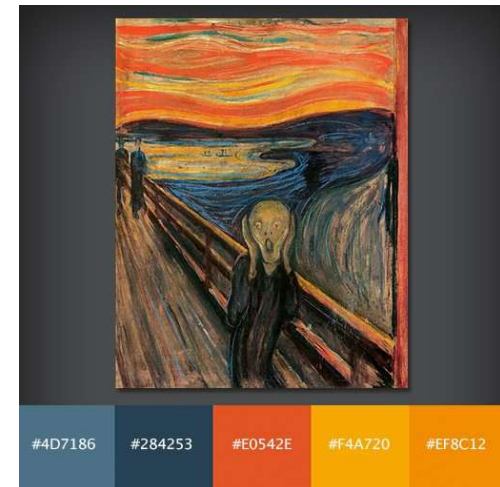
Schlieren and Color Palette?



The Great Wave, Hokusai



Starry Night, Vincent Van Gogh

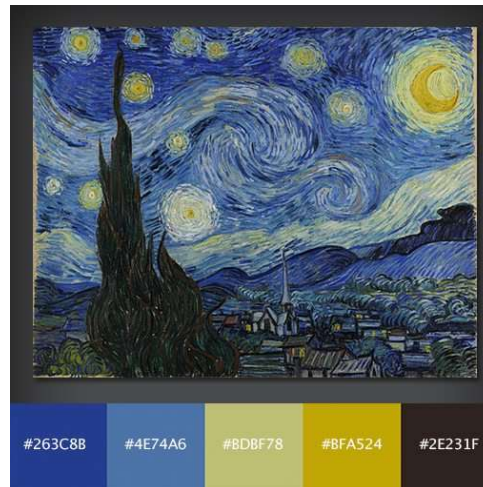
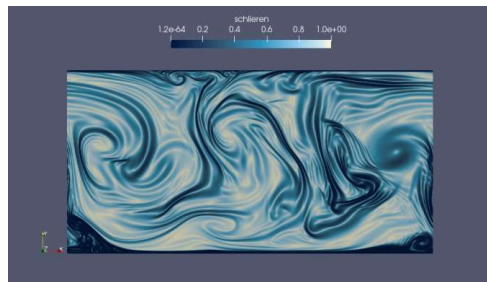


The Scream, Edvard Munch

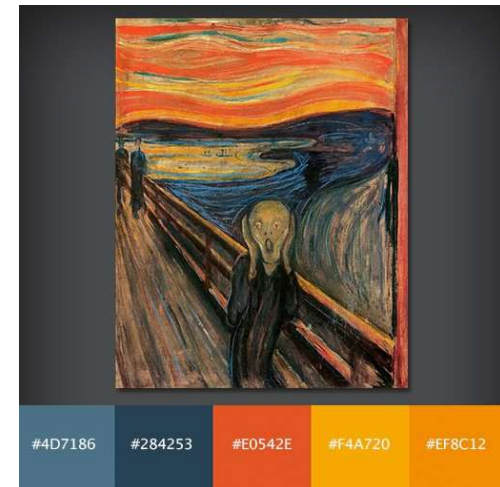
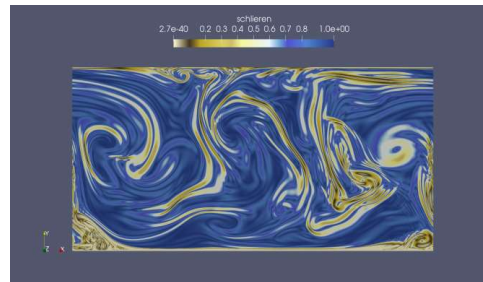
Schlieren and Color Palette!



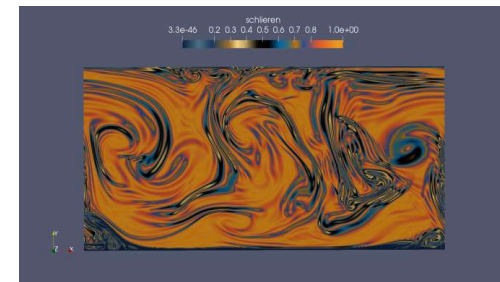
The Great Wave, Hokusai



Starry Night, Vincent Van Gogh



The Scream, Edvard Munch



Movie

- Of course, we made a movie...
- <https://youtu.be/1DIGnRgUhe4>
- If you are a music aficionado, please try to identify the soundtrack!
- Major respect to anyone who know the opus number, double bonus if you can guess the pianist.