# A numerical approach to Newtonian and viscoplastic free surface flows using dynamic octree meshes

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# Outline

- Models for Newtonian and viscoplastic fluid one-phase free-surface flow
- Level set method for free surface capturing
- Numerical scheme
  - Time integration
  - Mesh adaptation and discretization
  - Volume correction and reinitialization
- New advances in discretization of NS equations on octree meshes

## A model for free-surface viscous fluid flow

Fluid domain: $\Omega(t) \in \mathbb{R}^3$ with boundary $\overline{\partial\Omega(t)} = \overline{\Gamma_D} \cup \overline{\Gamma(t)}$
$\Gamma_D$: solid part, $\Gamma(t)$: free surface

Fluid equations:

$$\left\{ \begin{array}{r} \rho\left(\dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) - \mathbf{div}\,\boldsymbol{\tau} + \nabla p = \mathbf{f} \\ \nabla\cdot\mathbf{u} = 0 \end{array} \right. \quad \text{in } \Omega(t),$$

Newtonian fluid constitutive law

$$\boldsymbol{\tau} = \mu \mathbf{D}\mathbf{u}$$

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$\mu$: viscosity parameter,
$\rho$: density of fluid, $\mathbf{u}$: velocity vector, $p$: kinematic pressure,
$\mathbf{Du}$: rate of strain tensor,
$\boldsymbol{\tau}$: deviatoric part of the stress tensor

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The Herschel-Bulkley constitutive law

$$\begin{aligned} \boldsymbol{\tau} = \left(K\,|\mathbf{Du}|^{n-1} + \tau_s|\mathbf{Du}|^{-1}\right)\mathbf{Du} \;&\Leftrightarrow\; |\boldsymbol{\tau}| > \tau_s, \\ \mathbf{Du} = \mathbf{0} \;&\Leftrightarrow\; |\boldsymbol{\tau}| \le \tau_s. \end{aligned}$$

$K > 0$: consistency parameter, $\tau_s \ge 0$: yield stress parameter, $n > 0$: flow index,
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Note: Mathematically sound formulations are written in terms of variational inequalities (Duvaut, Lions 1976).

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Fluid equations (regularization):

$$\begin{cases} \rho \left( \dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) - \textbf{div}\, \mu_\varepsilon \mathbf{D}\mathbf{u} + \nabla p = \mathbf{f} \\ \nabla \cdot \mathbf{u} = 0 \end{cases} \quad \text{in } \Omega(t),$$

with the shear-dependent effective viscosity

$$\mu_\varepsilon = K\, |\mathbf{D}\mathbf{u}|_\varepsilon^{n-1} + \tau_s |\mathbf{D}\mathbf{u}|_\varepsilon^{-1}, \qquad |\mathbf{D}\mathbf{u}|_\varepsilon = \sqrt{|\mathbf{D}\mathbf{u}|^2 + \varepsilon^2}.$$

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Modeling error:

$$\|\mathbf{u}_0 - \mathbf{u}_\varepsilon\|_{H^1} \leq \sqrt{\varepsilon}$$

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Initial and boundary conditions:

$$\Omega(0) = \Omega_0, \quad \mathbf{u}|_{t=0} = \mathbf{u}_0 \quad \text{and} \quad \mathbf{u} = \mathbf{g} \quad \text{on } \Gamma_D.$$

---

$K > 0$: consistency parameter, $\tau_s \geq 0$: yield stress parameter, $n > 0$: flow index,
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Balance of the surface tension and stress forces:

$$(\mu_\varepsilon \mathbf{D}\mathbf{u} - p\,\mathbf{I})\mathbf{n}_\Gamma = \varsigma\kappa\mathbf{n}_\Gamma - p_{\text{ext}}\mathbf{n}_\Gamma \quad \text{on } \Gamma(t),$$

and kinematic condition on $\Gamma(t)$

$$v_\Gamma = \mathbf{u}|_\Gamma \cdot \mathbf{n}_\Gamma.$$

$K > 0$: consistency param., $\tau_s \geq 0$: yield stress param., $n > 0$: flow index,
$\rho$: density of fluid, $\mathbf{u}$: velocity vector, $p$: kinematic pressure,
$\mathbf{D}\mathbf{u}$: rate of strain tensor, $\varepsilon$: regularization param., $\mathbf{n}_\Gamma$: normal vector for $\Gamma(t)$,
$v_\Gamma$: normal velocity of $\Gamma(t)$, $\varsigma$: surface tension coef., $\kappa$: sum of principal curvature

# Interface capturing: Level set approach

**Idea:**(Sethian, Osher '87)

$$\Gamma(t) = \text{zero-level of a scalar function}$$

The level set function $\varphi(x,t)$

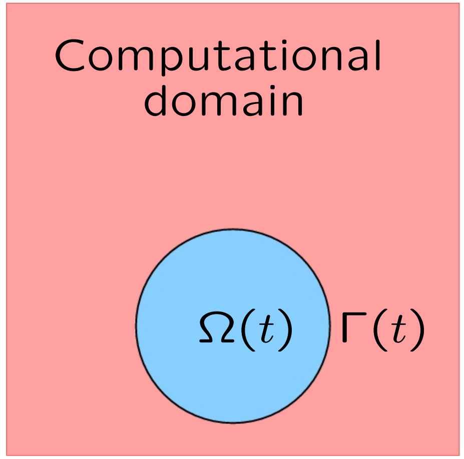
$$\phi(x,t) = \begin{cases} < 0 & \text{for } x \text{ in fluid domain } \Omega(t) \\ > 0 & \text{for } x \text{ in } \mathbf{R}^3 \setminus \Omega(t) \\ = 0 & \text{at the free surface} \end{cases}$$

should be an
*"approximate signed distance function"*.

$$x(t) \in \Gamma(t) \quad \Rightarrow \quad \phi(x(t),t) = 0.$$

Level set equation

$$\boxed{\phi_t + \widetilde{\mathbf{u}} \cdot \nabla \phi \quad = \quad 0 \quad \text{in} \quad \mathbb{R}^3}$$

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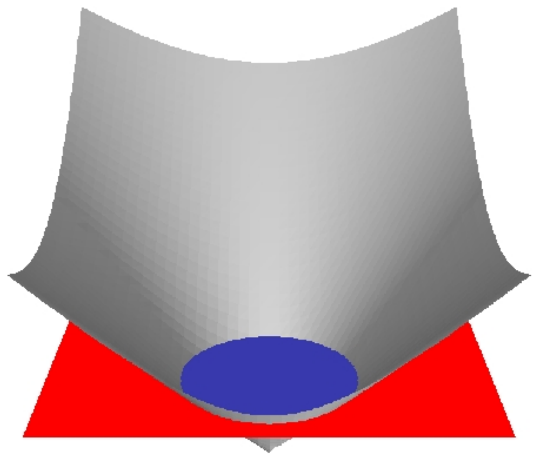

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$\Gamma_D$: solid part, $\Gamma(t)$: free surface

Fluid + level set equations + b.c. + i.c. (coupling between fluid and level set eqs. are in red):

$$\left\{\begin{aligned} \rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) - \mathbf{div}\,\mu_\varepsilon \mathbf{D}\mathbf{u} + \nabla p = \mathbf{f} \\ \nabla\cdot\mathbf{u} = 0 \\ \mu_\varepsilon = K\,|\mathbf{D}\mathbf{u}|_\varepsilon^{n-1} + \tau_s |\mathbf{D}\mathbf{u}|_\varepsilon^{-1} \end{aligned}\right. \quad \text{in } \Omega(t),$$

$$\mathbf{u}|_{t=0} = \mathbf{u}_0 \quad \text{and} \quad \mathbf{u} = \mathbf{g} \quad \text{on } \Gamma_D, \quad (\mu_\varepsilon \mathbf{D}\mathbf{u} - p\,\mathbf{I})\mathbf{n}_\Gamma = \varsigma\kappa\mathbf{n}_\Gamma \quad \text{on } \Gamma(t)$$

$$\left\{\begin{aligned} \frac{\partial \phi}{\partial t} + \widetilde{\mathbf{u}}\cdot\nabla\phi = 0 \quad & \text{in } \mathbb{R}^3 \times (0,T] \\ \phi(0) = \phi_0, & \end{aligned}\right.$$

with $\mathbf{n}_\Gamma = \nabla\phi/|\nabla\phi|$, and $\kappa = \nabla\cdot\mathbf{n}_\Gamma$.

Distance property: $|\nabla\phi| = 1$.

$K > 0$: consistency param., $\tau_s \geq 0$: yield stress param., $n > 0$: flow index,
$\rho$: density of fluid, $\mathbf{u}$: velocity vector, $p$: kinematic pressure,
$\mathbf{D}\mathbf{u}$: rate of strain tensor, $\varepsilon$: regularization param., $\mathbf{n}_\Gamma$: normal vector for $\Gamma(t)$,
$v_\Gamma$: normal velocity of $\Gamma(t)$, $\varsigma$: surface tension coef., $\kappa$: sum of principal curvature

# Numerical method

Loop:

1. *Level set part*: $\Omega(t) \to \Omega(t + \Delta t)$
2. *Remeshing*
3. *Re-interpolation*
4. *Fluid part*: $\{\mathbf{u}(t), p(t)\} \to \{\mathbf{u}(t + \Delta t), p(t + \Delta t)\}$

end of the loop.

# Numerical method

Loop:

1. *Level set part*: $\Omega(t) \to \Omega(t + \Delta t)$
   (a) Extend the velocity along normals to $\Gamma(t)$, $\mathbf{u}(t)|_{\Omega(t)} \to \widetilde{\mathbf{u}}(t)|_{\mathbb{R}^3}$:
   $$\mathbf{y}^0 = \mathbf{x}, \quad \mathbf{y}^{n+1} = \mathbf{y}^n - \alpha\phi_h(\mathbf{y}^n)\nabla\phi_h(\mathbf{y}^n), \quad \text{until } |\mathbf{y}^{n+1} - \mathbf{y}^n| \le \varepsilon$$
   set $u_h(\mathbf{x}) = u_h(\mathbf{y}^{n+1})$.
   (b) Semi-Lagrangian step for $\frac{\partial\phi}{\partial t} + \widetilde{\mathbf{u}} \cdot \nabla\phi = 0$
   (c) Volume correction: Solve for $\delta$: meas$\{\mathbf{x} : \phi(\mathbf{x}) < \delta\} = Vol^{\text{reference}}$ and correct $\phi^{new} = \phi - \delta$
   (d) Update $\phi$ to satisfy $|\nabla\phi| = 1$: Invokes The Marching Cubes method (Lorensen & Cline, 1987)
2. *Remeshing*
3. *Re-interpolation*
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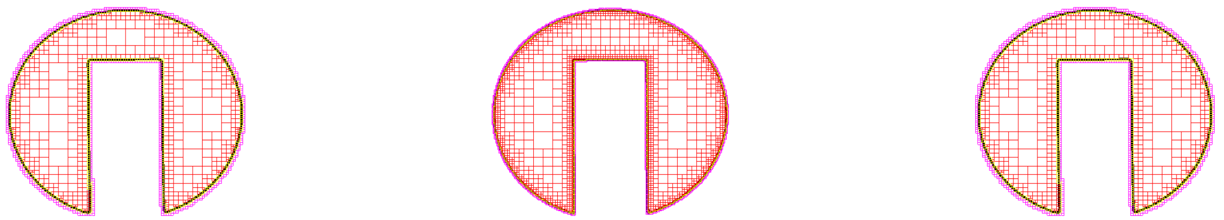
   (b) Semi-Lagrangian step for $\frac{\partial \phi}{\partial t} + \widetilde{\mathbf{u}} \cdot \nabla \phi = 0$

   Zalesak's test: advection by a prescribed velocity field
   2-nd order semi-Lagrangian and enhanced with particle-level set



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# Numerical method

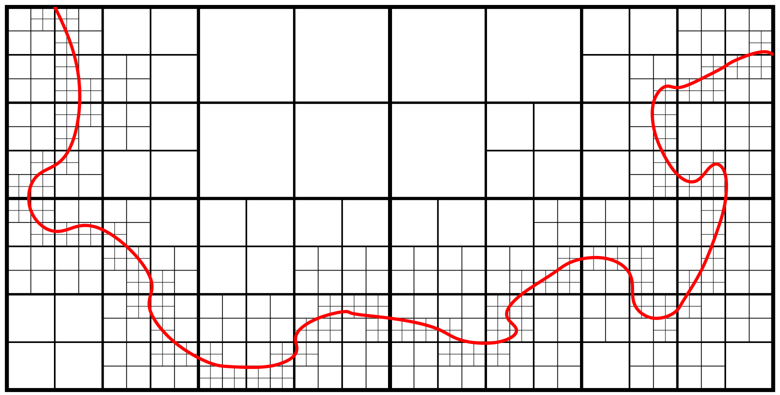
Loop:

1. *Level set part*: $\Omega(t) \to \Omega(t + \Delta t)$

2. *Remeshing*:

   (a) Graded octree cartesian mesh gradely adapted to $\Gamma(t + \Delta t)$ location.

   (b) 2D Illustration:



3. *Re-interpolation*

4. *Fluid part*: $\{\mathbf{u}(t), p(t)\} \to \{\mathbf{u}(t + \Delta t), p(t + \Delta t)\}$

end of the loop.

# Numerical method

Loop:

1. *Level set part*: $\Omega(t) \to \Omega(t + \Delta t)$

2. *Remeshing*

3. *Re-interpolation*

   (a) trilinear interpolation in cubic cells

   (b) Semi-Lagrangian methods and upwind differences also use higher order interpolation

4. *Fluid part*: $\{\mathbf{u}(t), p(t)\} \to \{\mathbf{u}(t + \Delta t), p(t + \Delta t)\}$

end of the loop.

# Numerical method

Loop:

1. *Level set part*: $\Omega(t) \to \Omega(t + \Delta t)$

2. *Remeshing*

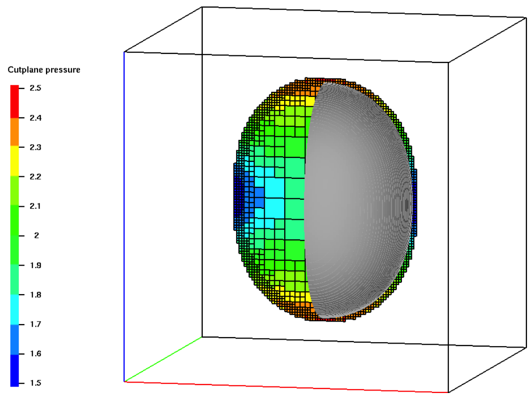
3. *Re-interpolation*

4. *Fluid part*: $\{\mathbf{u}(t), p(t)\} \to \{\mathbf{u}(t + \Delta t), p(t + \Delta t)\}$
   (a) Staggered location of pressure-velocity nodes
   (b) Chorin-Yanenko type splitting:
      - Semi-Lagrangian meth. for advection
      - For (explicit) visco-plastic step we discretize
        $$\textbf{div}\, \mu_\varepsilon \mathbf{D}\mathbf{u} = \frac{1}{2}\left(\textbf{div}\, \mu_\varepsilon \nabla \mathbf{u} + (\nabla \mathbf{u})^T \nabla \mu_\varepsilon\right) \quad \text{(holds if } \nabla \cdot \mathbf{u} = 0\text{)}$$
        by a hybrid of meshless finite point and finite difference approaches.
      - Curvature evaluation $\kappa = \nabla \cdot \nabla\phi / |\nabla\phi|$
      - Standard projection (pressure-correction) step with
        $$p(t + \Delta t) = \varsigma\kappa(t + \Delta t) + p_{\text{ext}} \quad \text{on } \Gamma(t + \Delta t)$$

end of the loop.

# Computations for Newtonian fluid

*Freely oscillating droplet problem.*




Initial shape:

$$r = r_0(1 + \tilde{\varepsilon} S_2(\frac{\pi}{2} - \theta)),$$

$S_2$: second spherical harmonic, $r_0 = 1$,
Surface tension: $\varsigma = 1$, $\tilde{\varepsilon} = 0.3$, $K = 1/150$.

Energy balance for Newtonian fluid:

$$\frac{1}{2}\int_{\Omega(t)} |\mathbf{u}(t)|^2 \mathrm{d}\mathbf{x} + K \int_0^t \int_{\Omega(t)} |\mathbf{D}\mathbf{u}|^2 \,\mathrm{d}\mathbf{x}\,\mathrm{d}t' + |\Gamma(t)| = \frac{1}{2}\int_{\Omega(t)} |\mathbf{u}(0)|^2 \mathrm{d}\mathbf{x} + |\Gamma(0)|,$$

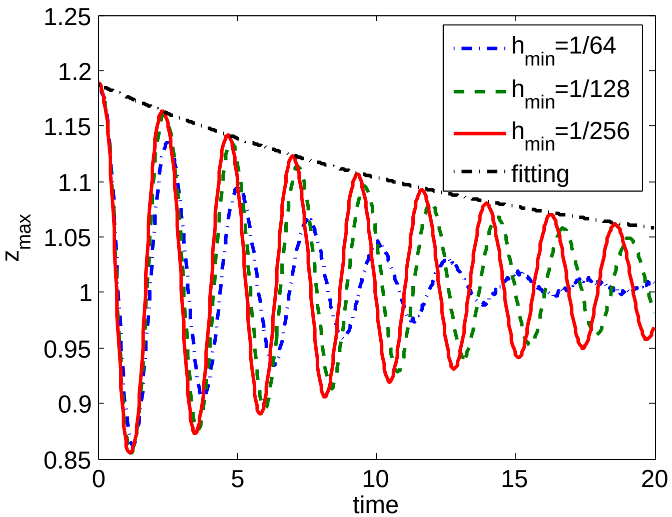
here $|\Gamma(t)| = meas(\Gamma(t))$.

For the Newtonian case:

Top tip trajectories on $z$ axes

and

fitting curve $z = r_\infty + c\,\exp(-\frac{t}{\delta})$
with $\delta = 16.2 \quad \Rightarrow \quad$ numerical dissipation is an issue.



# **Computations for <u>Herschel-Bulkley</u> fluid, $n = 1 \Rightarrow$ Bingham**

*Freely oscillating droplet problem.*

Viscoplastic case, $\tau_s > 0$

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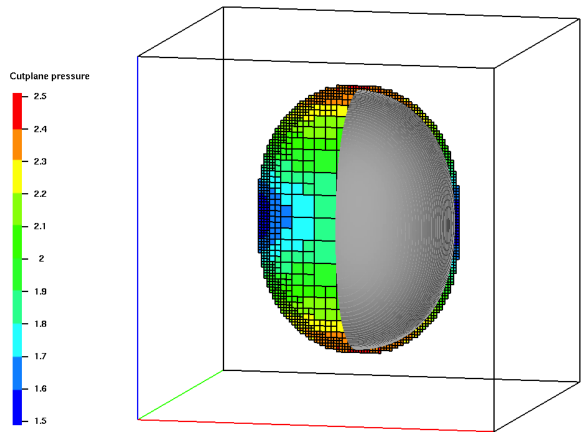
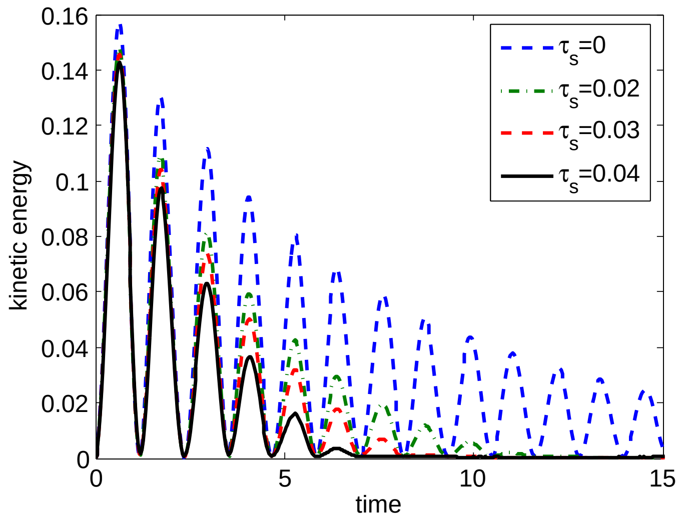
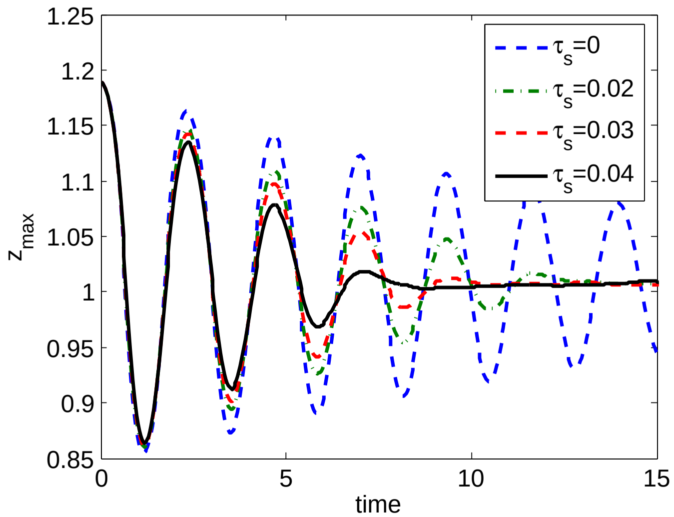
Finite cessation times?




The kinetic energy decay (left) and top tip trajectories (right) for different stress yield parameter values, $\tau_s \in \{0,\ 0.02,\ 0.03,\ 0.04\}$.



Numerical analysis challenge:

For the explicit time stepping treatment of visco-plastic term $\mathbf{div}\mu_\varepsilon\mathbf{Du}$ one might expect stability condition:

$$\Delta t \le \frac{h^2_{\mathsf{min}}}{\mathsf{max}\,|\mu_\varepsilon|}, \qquad (\text{in practice } \mathsf{max}\,|\mu_\varepsilon| \gtrsim 10^7).$$

Was not observed in practice!

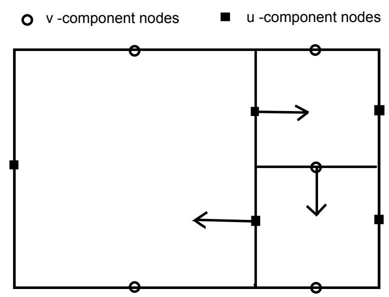
Observed stability can be related with the non-linear dependence of $\mu_\varepsilon$ on $\mathbf{u}$ (for large $\mu_\varepsilon$ the solution is constrained)...
More rigorous explanation would be very desirable.

## New advances in discretization of NS equations on octree meshes

- FV on staggered grids with high order FD for diffusion and advection fluxes
- Interpolation operators with compact stencils
- Damping divergence free parasitic modes by a low-pass filter

$$G \circ u(\mathbf{x}) = \begin{cases} \frac{1}{4}\sum_{i=1}^{4} u(\mathbf{x}_i) & \text{if } \mathbf{x} \in \Gamma_{cf}, \\ u(\mathbf{x}) & \text{otherwise,} \end{cases}$$

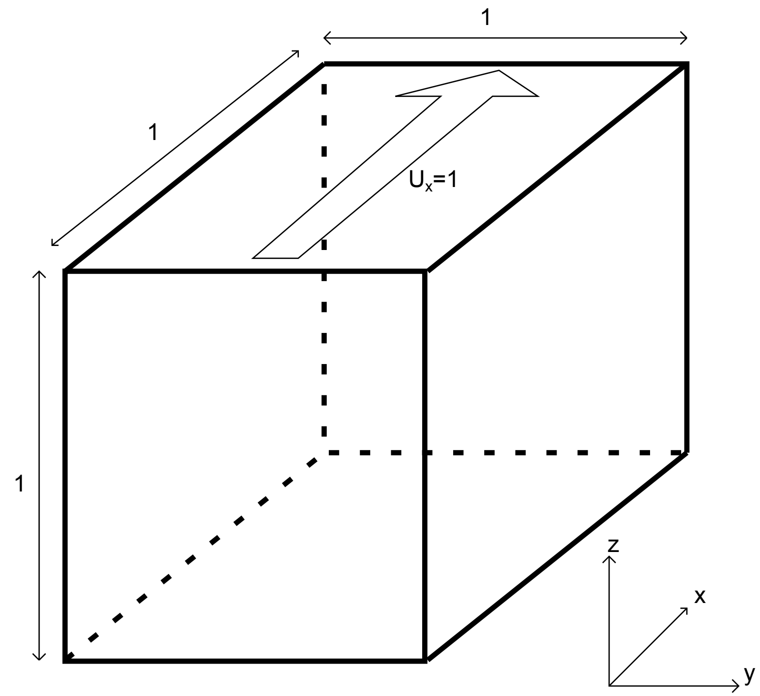
$$... + G \circ \mathbf{u}^n \cdot \nabla \mathbf{u}^{n+1} ....$$

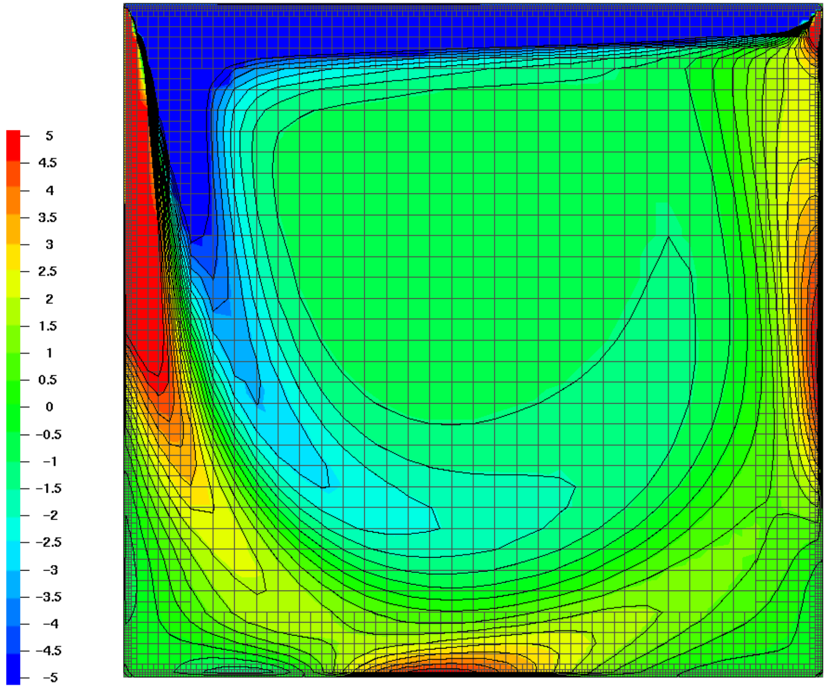


divergence free mode

Y.V.,M.O.,K.T., Computers and Fluids, 84 (2013) 231-246.

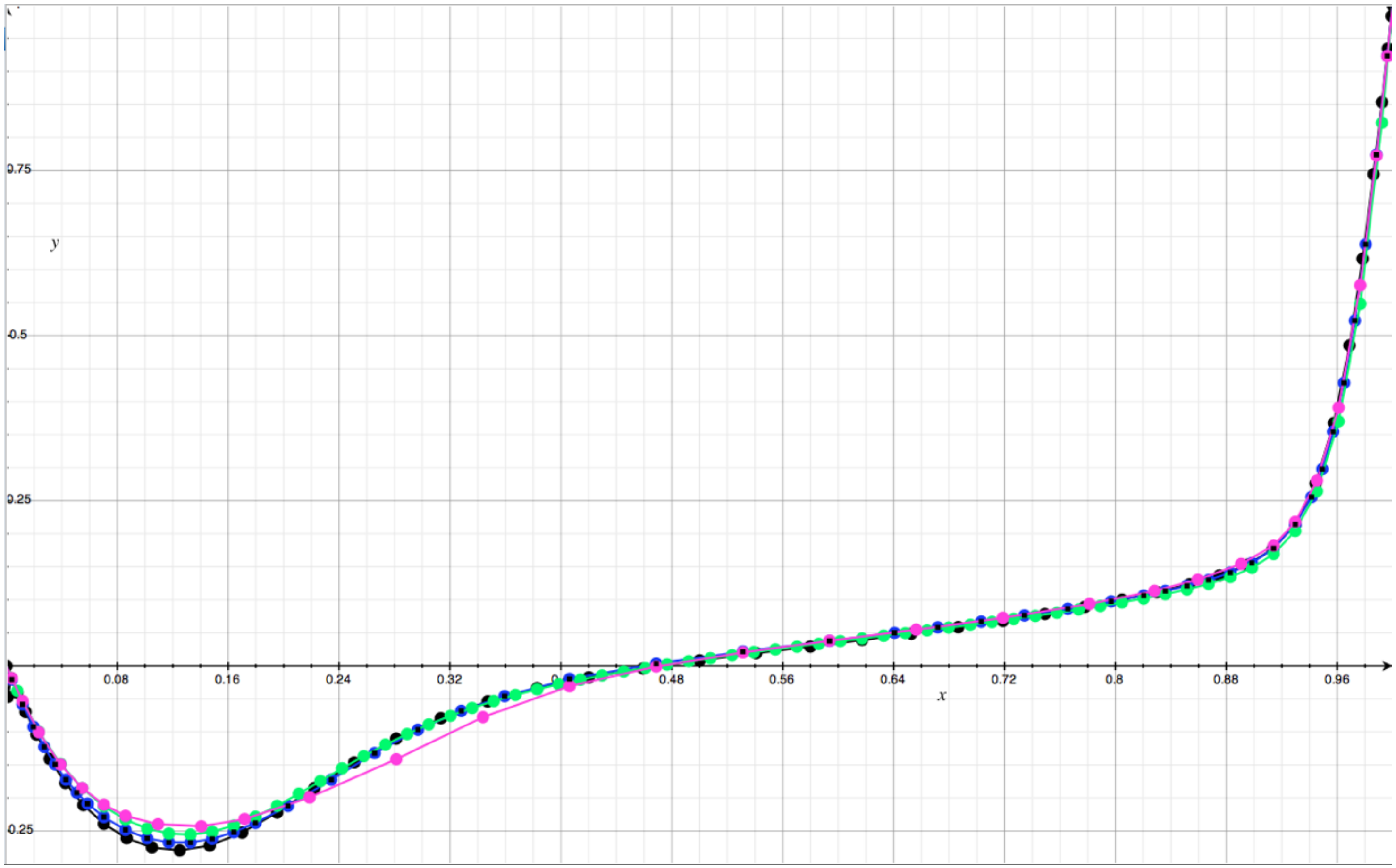
# 3D cavity problem, Re = 1000




Spanwise vorticity for the midplane $y = 0.5$

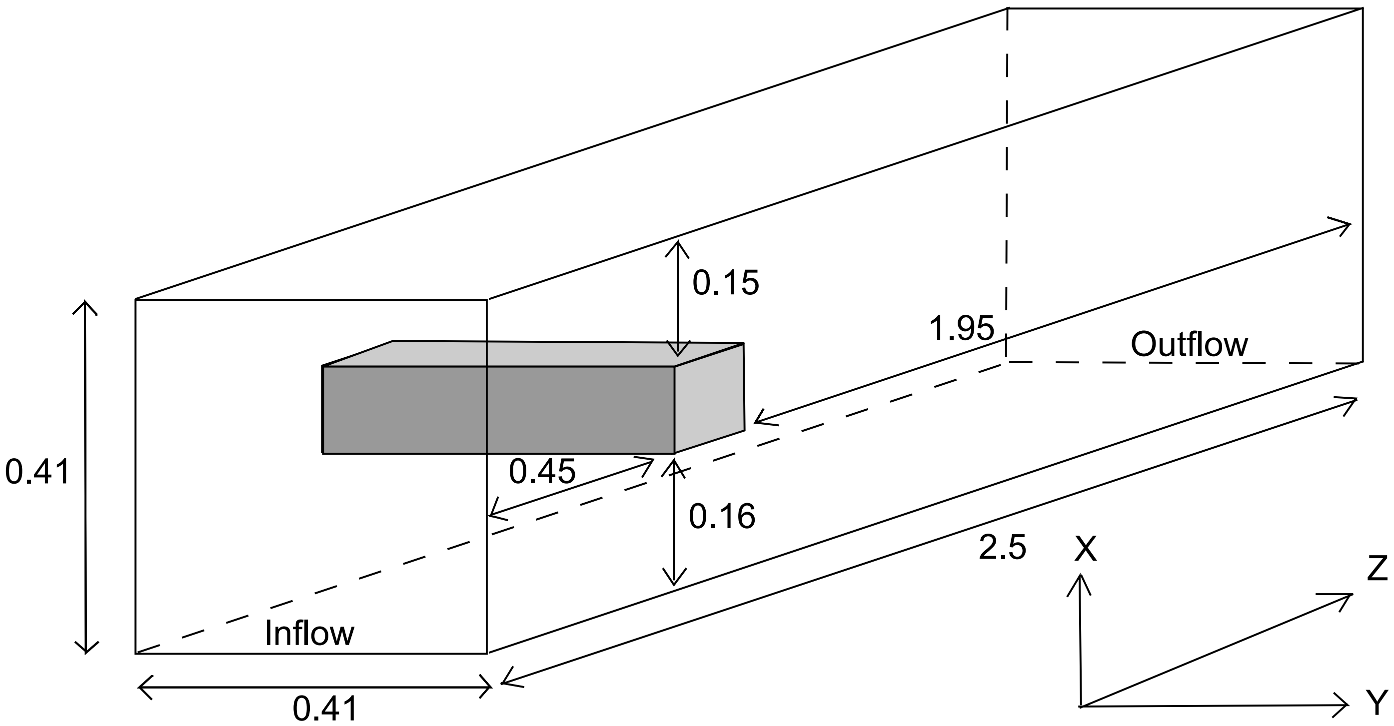
# 3D cavity problem, Re = 1000




The centerline $((0.5, 0.5, z),\ \ 0 \leq z \leq 1)$, $u_x$-velocities

- Black: Wong-Backer
- Green: 64x64x64
- Pink: refinement 128-16
- Blue: refinement 128-32

# 3D flow around a square cylinder, Re=100



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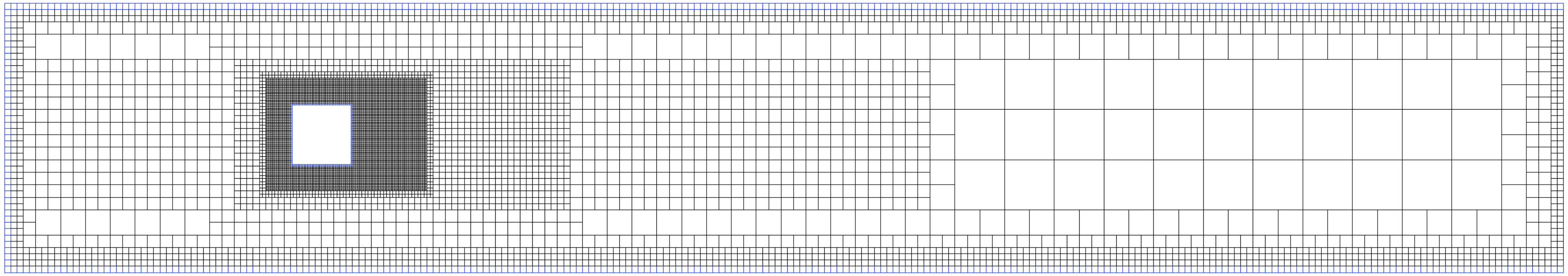
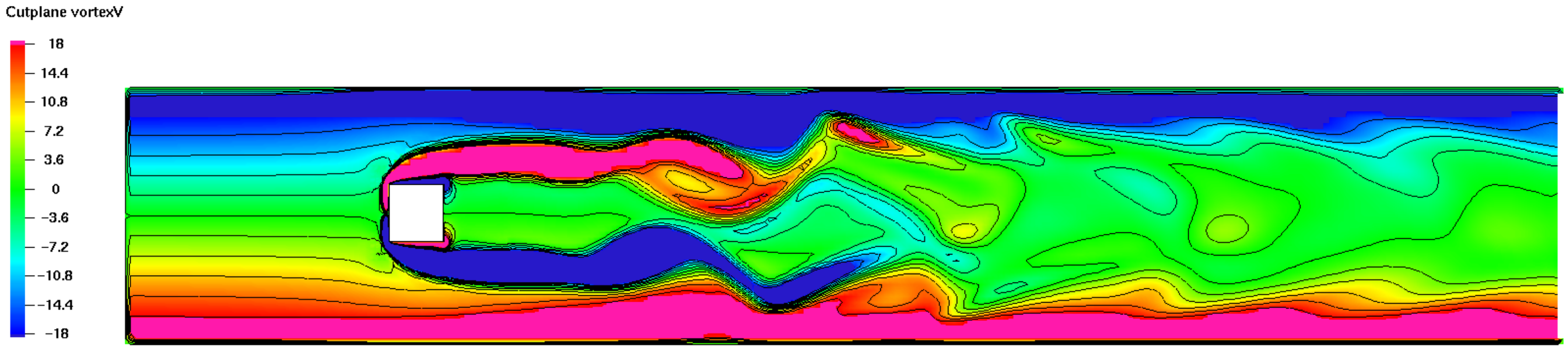


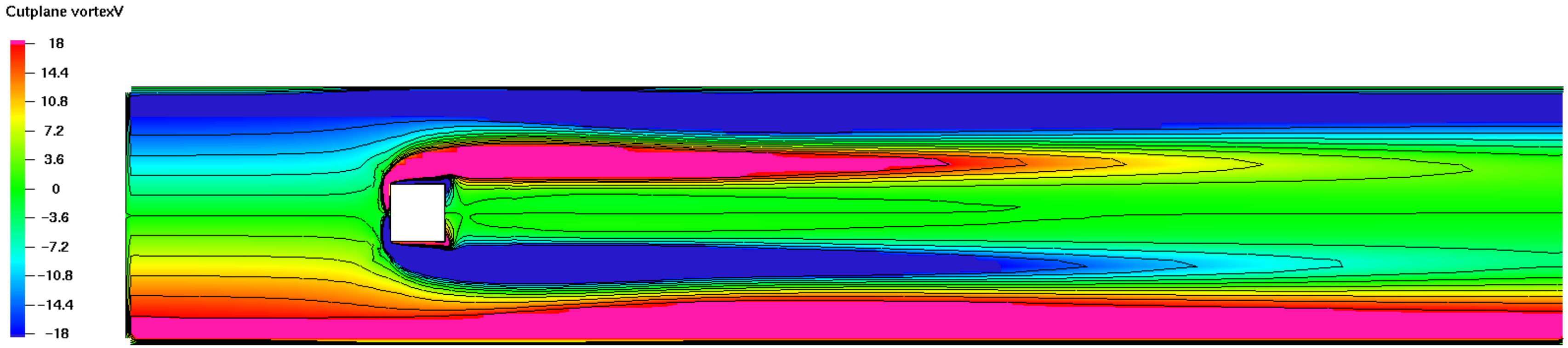
| $h_{min}$ | $h_{max}$ | $C_{\text{drag}}$ | $C_{\text{lift}}$ | St |
|---|---|---|---|---|
| 1/256 | 1/256 | 6.204 | 0.07631 | $*$ |
| 1/512 | 1/256 | 5.222 | 0.04407 | 0.326 |
| 1/1024 | 1/256 | 4.679 | 0.02697 | 0.297 |
| 1/2048 | 1/256 | 4.484 | 0.03166 | 0.307 |
| Schafer & Turek | | 4.32–4.67$^\dagger$ | 0.015–0.05$^\dagger$ | 0.27–0.35$^\dagger$ |
| 1/1024 | 1/32 | 4.671 | 0.02666 | 0.306 |

$*$ Solution has not attained a periodic regime for $t \in [0, 16]$.

† Reference intervals may be not very accurate.

# 3D flow around a square cylinder, Re=100

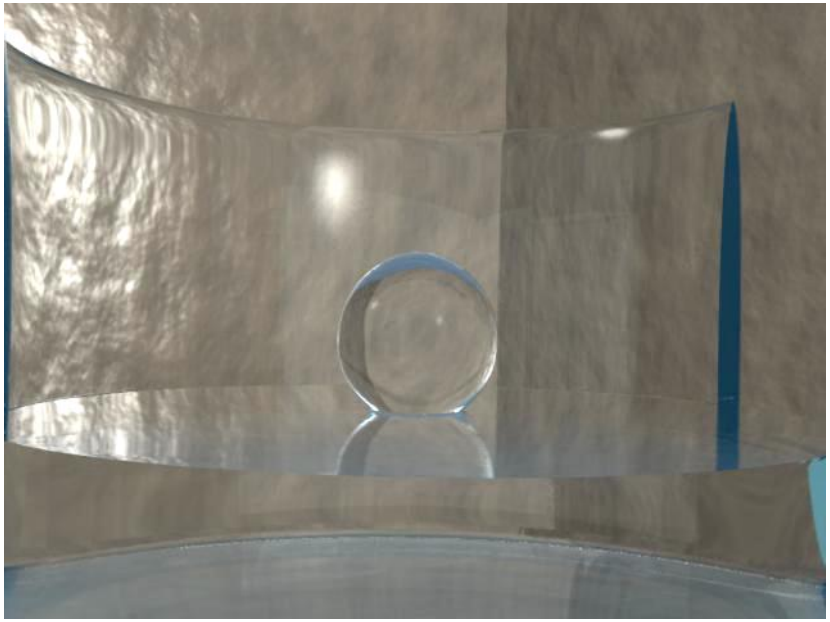


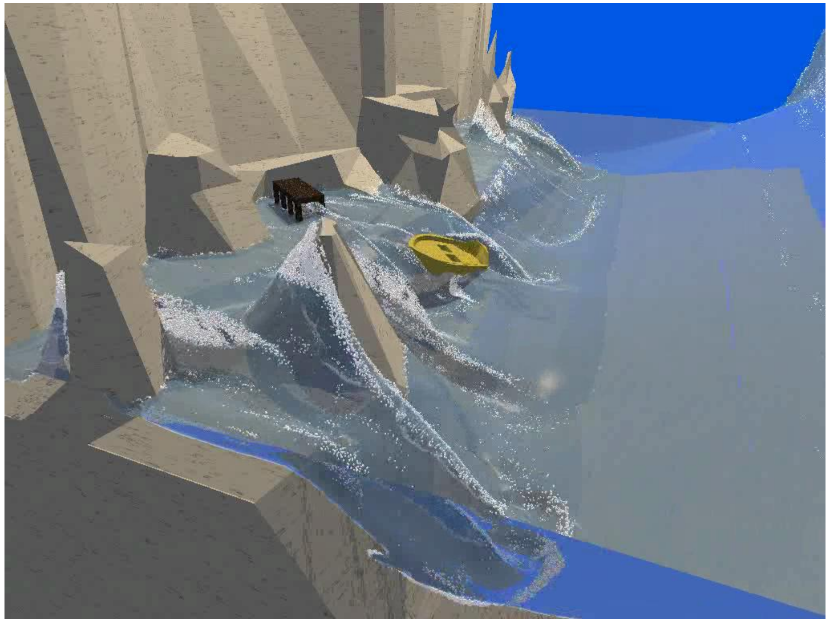



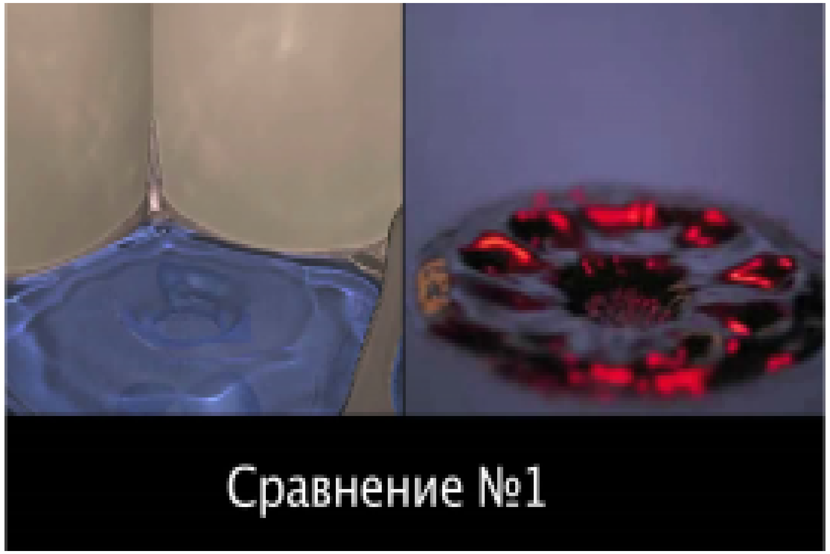

Advective terms: FV versus semi-Lagrangian method (linear interpolation).

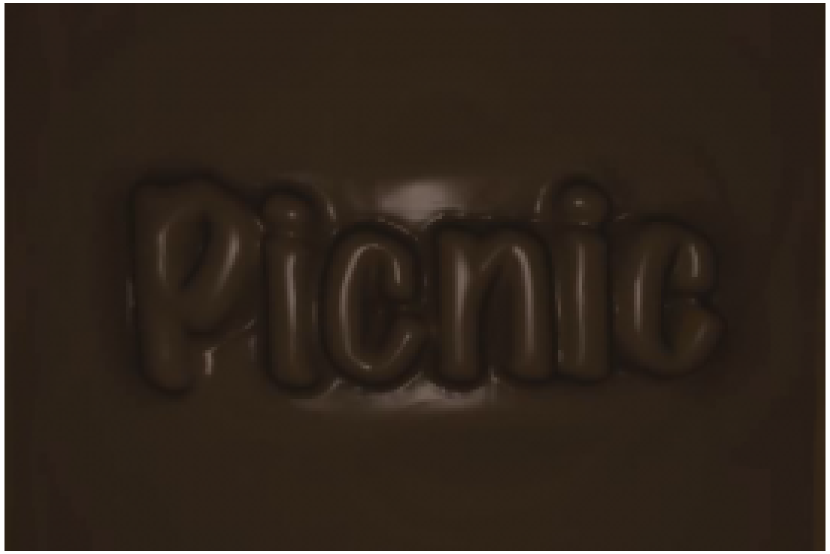
Spanwise vorticity at time t=16 for the midplane $y = 0.205$, $h_{\text{max}} = 1/256$, $h_{\text{min}} = 1/1024$.

# Newtonian fluid

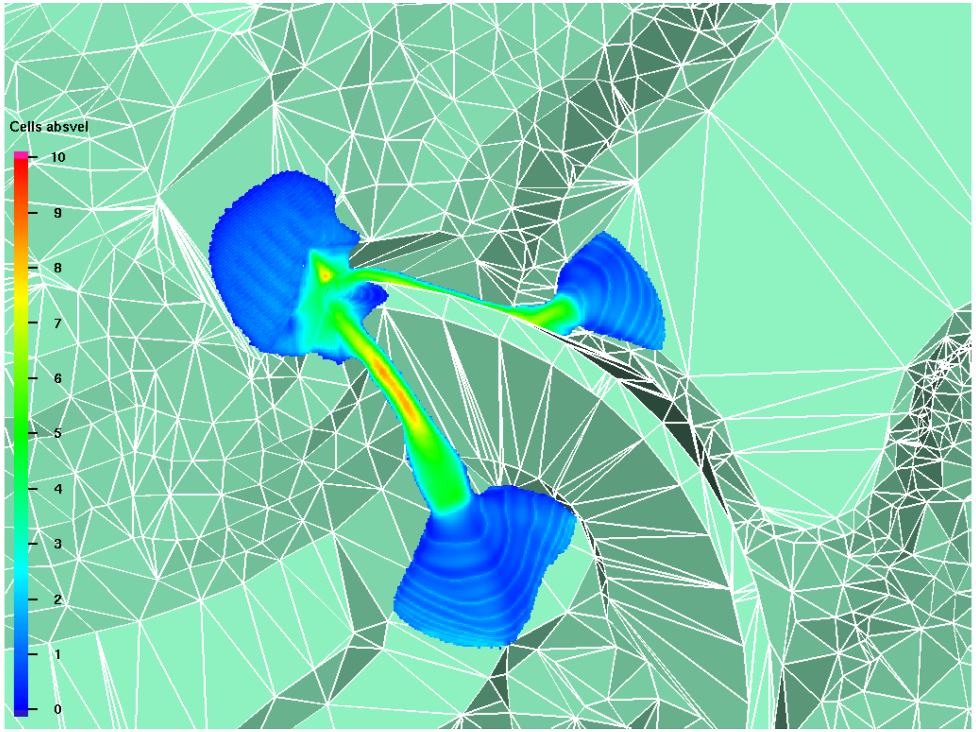


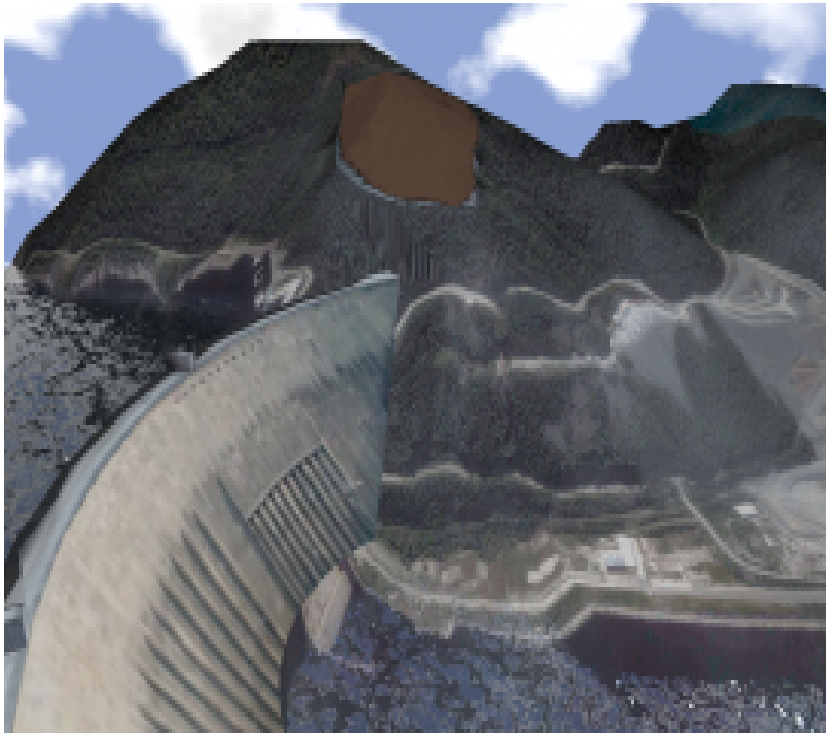


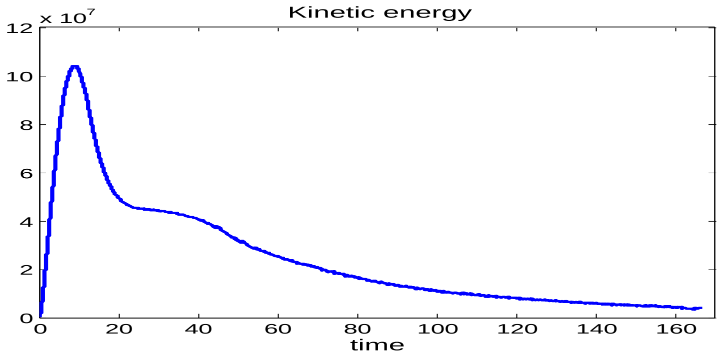


## Sayano-Shushenskaya Dam Landslide (real-life topography)





Much more (papers, flows animations) on:

www.inm.ras.ru/research/freesurface

Research project MSE on mathematical modeling of natural disasters and technical hazards (2011-2013)

- Energy inequality:

$$\frac{1}{2}\int_{\Omega(t)}\rho|\mathbf{u}(t)|^2\mathrm{d}\mathbf{x}+\int_0^t\int_{\Omega(t)}K|\mathbf{Du}|^{1+n}+\tau_s|\mathbf{Du}|\,\mathrm{d}\mathbf{x}\,\mathrm{d}t'+\varsigma|\Gamma(t)|$$
$$\leq\frac{1}{2}\int_{\Omega(t)}\rho|\mathbf{u}(0)|^2\mathrm{d}\mathbf{x}+\int_0^t\int_{\Omega(t)}\mathbf{f}\,\mathbf{u}\,\mathrm{d}\mathbf{x}\,\mathrm{d}t'+\varsigma|\Gamma(0)|,$$

  here $|\Gamma(t)| = meas_{R^2}(\Gamma(t))$.

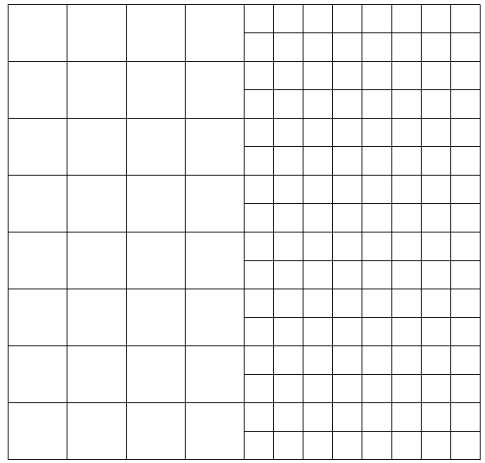
  Note: This becomes energy equality (energy balance) for $\varepsilon > 0$, with $\int_0^t\int_{\Omega(t)}\mu_\varepsilon|\mathbf{Du}|^2$ standing for the dissipation term.

- Mass conservation.

- Volume conservation.

- Plug and yield regions.(?)

"Instability" of Helmholtz decomposition



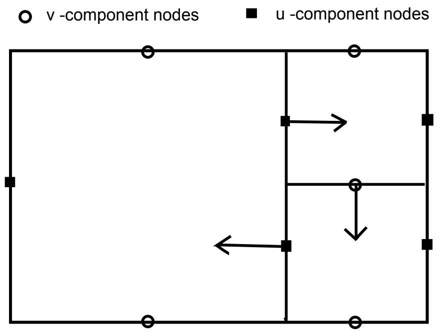
$$\begin{cases} \mathbf{f} = \mathbf{u} + \nabla p, \\ \mathbf{div}\mathbf{u} = 0, \\ \mathbf{u}\cdot\mathbf{n}|_{\partial\Omega} = \mathbf{f}\cdot\mathbf{n}|_{\partial\Omega}. \end{cases} \iff \begin{cases} -\mathbf{div}\nabla p = \mathbf{div}\mathbf{f}, \\ \left.\dfrac{\partial p}{\partial \mathbf{n}}\right|_{\partial\Omega} = 0, \\ \mathbf{u} = \mathbf{f} - \nabla p. \end{cases}$$

$$u = \sin\left(\frac{2\pi(e^x-1)}{e-1}\right)\left(1-\cos\left(\frac{2\pi(e^{ay}-1)}{e^a-1}\right)\right)\frac{1}{2\pi}\frac{e^x}{(e-1)},$$

$$v = \left(1-\cos\left(\frac{2\pi(e^x-1)}{e-1}\right)\right)\sin\left(\frac{2\pi(e^{ay}-1)}{e^a-1}\right)\frac{a}{2\pi}\frac{e^{ay}}{(e^a-1)},$$

$$p = a\cos\left(\frac{2\pi(e^x-1)}{e-1}\right)\cos\left(\frac{2\pi(e^{ay}-1)}{e^a-1}\right)\frac{e^{a+1}}{(e-1)(e^a-1)},$$

| quantity | mesh size $h$ | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 1/8 | 1/16 | 1/32 | 1/64 | 1/8 | 1/16 | 1/32 | 1/64 |
| | uniform mesh | | | | locally refined mesh | | | |
| $\|\mathbf{u}-\mathbf{u}_h\|_{L^\infty}$ | 1.1e-1 | 2.9e-2 | 1.1e-2 | 3.8e-3 | 1.4e-1 | 7.0e-1 | 3.5e-1 | 1.8e-1 |




divergence free mode

Low-pass filter

$$\begin{cases} \mathbf{f} = (I - \alpha h^2 \Delta_\Gamma)\mathbf{u} + \nabla p, \\ \mathbf{div}\mathbf{u} = 0, \\ \mathbf{u} \cdot \mathbf{n}|_{\partial\Omega} = \mathbf{f} \cdot \mathbf{n}|_{\partial\Omega}. \end{cases}$$

$\Delta_\Gamma$ is the vector Laplace-Beltrami op. $\Gamma_{cf}$

| quantity | mesh size $h$ | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 1/8 | 1/16 | 1/32 | 1/64 | 1/8 | 1/16 | 1/32 | 1/64 |
| | no filter | | | | low-pass filter | | | |
| $\|\mathbf{u} - \mathbf{u}_h\|_{L^\infty}$ | 1.4e-1 | 7.0e-1 | 3.5e-1 | 1.8e-1 | 1.2e-1 | 4.9e-1 | 2.2e-2 | 1.0e-2 |

$$G \circ u(\mathbf{x}) = \begin{cases} \frac{1}{4}\sum_{i=1}^{4} u(\mathbf{x}_i) & \text{if } \mathbf{x} \in \Gamma_{cf}, \\ u(\mathbf{x}) & \text{otherwise,} \end{cases}$$

$$... + G \circ \mathbf{u}^n \cdot \nabla \mathbf{u}^{n+1} ....$$