Numerical approximation of statistical solutions of incompressible flows

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Content

What do we want to compute?

Consider the incompressible Navier-Stokes equations (NSE):

$$\mathbf{U}_t + \nabla \cdot (\mathbf{U} \otimes \mathbf{U}) + \nabla p = \nu \Delta \mathbf{U} + f \quad (1)$$

$$\nabla \cdot \mathbf{U} = 0 \quad (2)$$

- $\mathbf{U}$ is the velocity
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and the (formal) vorticity formulation:

$$\eta_t + (\mathbf{U} \cdot \nabla)\eta - (\eta \cdot \nabla)\mathbf{U} = \nu \Delta \eta + g \quad (3)$$

$$\eta = \mathrm{curl}\ \mathbf{U} \quad (4)$$

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Goal: *define and approximate* suitable notion of **statistical solutions**.

State of the art for individual solutions

Mathematically:

- local existence of classical solutions
- global existence of *weak solutions* [Leray, 1934, Hopf, 1950]
- in general: no regularity/uniqueness results (1M$ problem)

$\Rightarrow$ incomplete understanding

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Numerically:

- computationally intensive
- statistical sampling usually requires a *large number of simulations*

$\Rightarrow$ very expensive simulations
$\Rightarrow$ need supercomputers

Piz Daint. Source: CSCS

Why do we want to compute statistical solutions?

Statistical approach may help and is widely used, e.g.

- Reynolds Averaged Navier-Stokes (RANS):
  in engineering, formal averaging of NSE
- measure valued solutions (MVS) for Euler:
  attempt to make sense of the vanishing viscosity limit
- statistical solutions:
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All concepts are related but focused on different goals.

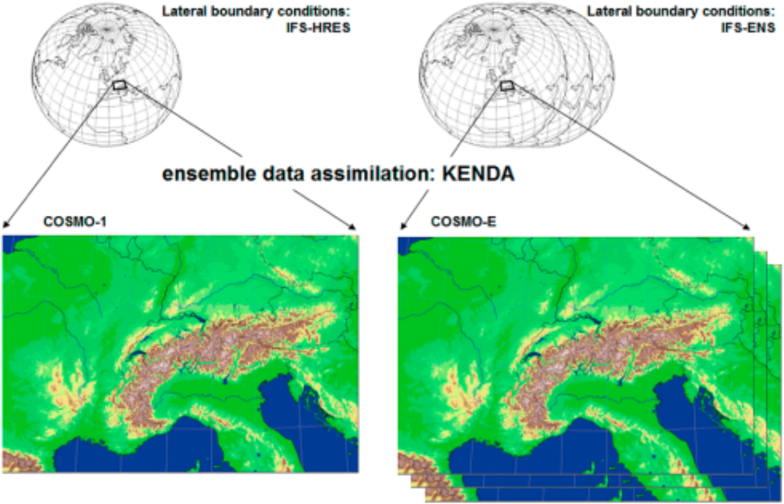
Here, we focus on statistical solutions.

Motivational example: weather prediction

(Numerical) weather prediction uses **statistical sampling**:

- e.g. *COSMO-NExT* is the *state of the art* at *MeteoSwiss*

Motivational example: weather prediction



Future of numerical weather forecast at MeteoSwiss. Source: MeteoSwiss

Motivational example: weather prediction

(Numerical) weather prediction uses **statistical sampling**:

- e.g. *COSMO-NExT* is the *state of the art* at *MeteoSwiss*
- number of samples that can be used for everyday simulations: **20**
- if you ever ran a MC simulation you know that **this is not great**

What can be done to improve this?

Let's start simple...

For now we limit ourselves to:

- **viscous case**: Euler equations ($\nu = 0$) are much worse than NSE
- **periodic BCs**: no boundary layer effect
- **2d case**
  - vorticity is a scalar, orthogonal to the 2d plane;
  - no vortex stretching $(\eta \cdot \nabla)\mathbf{U} = 0$
  - $\Rightarrow$ vorticity remains bounded
  - $\Rightarrow$ well behaved solution [Ladyzhenskaya, 1969, Beale et al., 1984]
- **no vortex sheets** (vorticity is a Dirac mass on a curve): $\eta \in L^\infty$

However, we keep an eye on general case.

Defining a statistical solution

- If $\exists$ flow map $S^{\nu}(t)$, s.t. $\mathbf{U}(t) = S^{\nu}(t)(\mathbf{U}_0)$ and
- we have an initial measure μ_0, we can define μ_t^{ν}:

$$\mu_t^{\nu}(E) := \mu_0(S^{\nu}(t)^{-1}(E)), \quad \forall E \in \mathcal{B}(H), \tag{5}$$

  where H is a suitable solution space.
- [Foiaș and Prodi, 1976] proved: if $\int_H \|\mathbf{U}\|_H^2 d\mu_0(\mathbf{U}) < \infty$ then:
  1. a suitable notion of μ_t^{ν} **exists**
  2. (with constant forcing in 2D) is **unique and has the form** (5).

Vorticity reformulation

We did the same for the **vorticity formulation**:

1. if $T^\nu(t) := \mathrm{rot} \circ S^\nu(t) \circ \mathrm{rot}^{-1}$ is the vorticity flow map and
2. π_0 is an initial vorticity measure, we define

$$\pi_t^\nu(E) := \pi_0(T^\nu(t)^{-1}(E)) \tag{6}$$

Define the space: $V_s := \{u \in H^s(\mathbb{T}^2)^2 \mid \mathrm{div}\, u = 0, \int_{\mathbb{T}^2} u dx = 0\}$
For $s > 0$:

$$\begin{array}{ccc} V_{s+1} & \xrightarrow{S_t^\nu} & V_{s+1} \\ \downarrow \mathrm{rot} & & \downarrow \mathrm{rot} \\ H^s(\mathbb{T}^2) & \xrightarrow{T_t^\nu} & H^s(\mathbb{T}^2) \end{array} \tag{7}$$

Computing stat. sol.: what do we need?

- a single sample evolver (approximation of flow maps T^ν or S^ν)
  - we use finite difference/volume (**FD**/**FV**) for efficiency (and simplicity)
- a "statistical integrator"
  - **Monte Carlo** (MC) is the simplest
  - but is also terribly slow: $O(N^{-1/2})$

We must be efficient but won't sacrifice mathematical aspects.

The "deterministic" scheme

- **Vorticity formulation** [Levy and Tadmor, 1997]
- **Crank-Nicolson** time integration

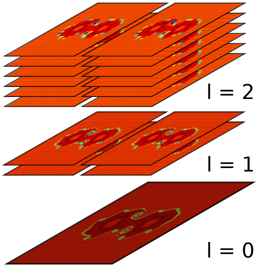
$$\frac{\eta^{n+1} - \eta^n}{\Delta t} = \mathbf{U}^n \nabla \left(\frac{\eta^{n+1} + \eta^n}{2} \right) + \nu \Delta \left(\frac{\eta^{n+1} + \eta^n}{2} \right) \tag{8}$$

Reconstruct $\mathbf{U}^n$ from η^n using the stream function ψ:

$$-\Delta \psi = \eta \quad \Rightarrow \quad \nabla^{\perp} \psi = \mathbf{U}, \quad \nabla \times \mathbf{U} = \eta. \tag{9}$$

- need a **Poisson solver** at each time iteration (heavy on wall-time)
- fortunately can be done (in theory) in $O(N)$ (multigrid)
- reconstruction $\mathbf{U}^n \Rightarrow$ scheme limited to formal $O(h)$

Multilevel Monte Carlo integration I



Idea: accelerate MC with multi-level (cf. multigrid) approach
l is coarsening level:

- l small: expensive computations, few samples
- l big: cheap computations, many samples

- introduced in [Giles, 2008] for SDEs
- hyperbolic conservation laws [Mishra et al., 2012, Barth et al., 2013]
- we call this **multi level Monte Carlo**

Multilevel Monte Carlo integration II

- more difficult to efficiently implement and parallelize
- MLMC requires (good) error bounds to outperform SLMC

Exploits **different levels of discretization** and the observation:

$$\mathbb{E}(X_0) = \sum_{l=0}^{L-1} \left(\mathbb{E}(X_l) - \mathbb{E}(X_{l+1})\right) + \mathbb{E}(X_L). \tag{10}$$

Error bounds I

If we are lucky, norm bounds look like [Majda and Bertozzi, 2002]:

$$\|\eta(t)\|_{H^m} \leq e^{(e^{C_m t}-1)} \|\eta_0\|_{H^m}^{(e^{C_m t})}, \ \forall m > 1$$

Notice:

- exponential in time: usually due to **Gronwall**
- constants are big, and grow with increasing regularity

$\Rightarrow$ numerically, we cannot hope for better.

Error bounds II

After a very long computation and a few Gronwall arguments:

$$\|\eta - \eta_{ex}\|_{L^2} \leq Kh(1 + C)\exp(C) \tag{11}$$

for η sufficiently smooth.

- K and C **depends (badly)** on high norms of η_0, final time and domain
- however, C does not depend on ν
- $K \to 1$ as $\nu \to \infty$
- K is bounded as $\nu \to 0$
- in particular, this holds also for Euler

Combining with MLMC algorithm:

$$\|E_{MLMC}[\eta] - \mathbb{E}[\eta_{ex}]\|_{L^2(\Omega;L^2(\mathbb{T}^2))} \leq \mathbb{E}[K(T, \eta_0)] \cdot (L + 1) \cdot h \tag{12}$$

Complexity

The magic of MLMC is the **reduction of wall-time**.

Work $\mathcal{W}$ and error $\mathcal{E}$ satisfy:

- single sample: optimally $\mathcal{E}_{det} \simeq \mathcal{W}_{det}^{-(1/3)}$
- SLMC: $\mathcal{E}_{SLMC} \simeq \mathcal{W}_{SLMC}^{-(1/5)}$
- MLMC: $\mathcal{E}_{MLMC} \simeq \mathcal{W}_{MLMC}^{-(1/3)}$, modulo a term L

MLMC has **complexity comparable** to that of a constant number of single samples.

The code

- written in **C++** (PETSc) and Python
- can use both SLMC and MLMC
- we use **domain decomposition** for parallelization
- computes SLMC/MLMC online and offline
- both vorticity and velocity formulations and different solvers
- computes individual solutions, stat. sol. and measure valued solutions
- geared towards experimentation
- runs on supercomputers (e.g. CSCS)

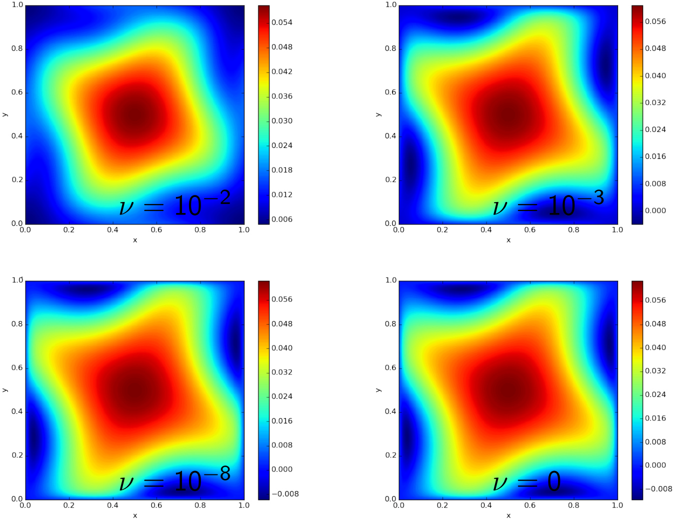
The code is (heavily) memory bound.

Experiment 1: Karhunen-Loève expansion I

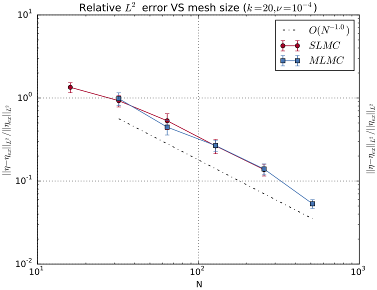
Initial vorticity mean given by:

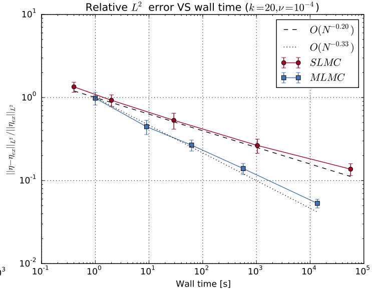
$$\bar{\eta}_0(x, y) := xy(1 - x)(1 - y)$$
$$\eta_0(\omega; x, y) := \bar{\eta}_0(x, y) + \sum_{(i,j)\in(\mathbb{Z}/M\mathbb{Z})^2} Y(\omega)_{i,j}(i + j)^{-2} \sin(\pi i x) \sin(\pi j y)$$

Experiment 1: Karhunen-Loève expansion II, plots



Experiment 1: Karhunen-Loève expansion III, error





Experiment 2: (smooth) shear layer I

A smooth shear layer is given by:

$$u_1(x,y) := \begin{cases} \tanh((x-0.25)/\rho) & x > 0.5 \\ \tanh((0.75-x)/\rho) & x \leq 0.5 \end{cases} \tag{13}$$

$$v_1(x,y) := \delta \sin(2\pi x) \tag{14}$$

ρ is the smoothing parameter (here 0.05)
δ is the small perturbation parameter

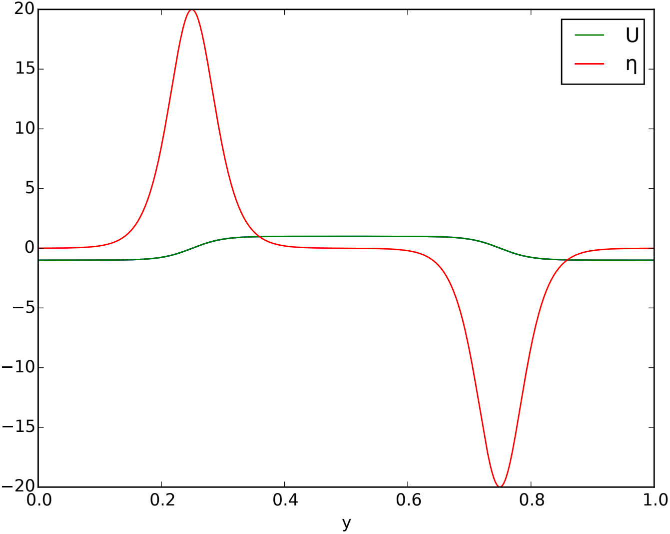
$$I(\omega, x) := \sum_{i \in \mathbb{Z}/M\mathbb{Z}} \delta Y(\omega)_{i,0} \sin(2\pi(x + Y(\omega)_{i,1})) \tag{15}$$

The uncertain smooth shear layer is given by:

$$(\tilde{u}_1, \tilde{u}_2)(\omega; x, y) := \mathbf{P}(u_1, u_2)(\omega, x, I(y)) \tag{16}$$

P is the Leray projector

Experiment 2: (smooth) shear layer I, mean and variance



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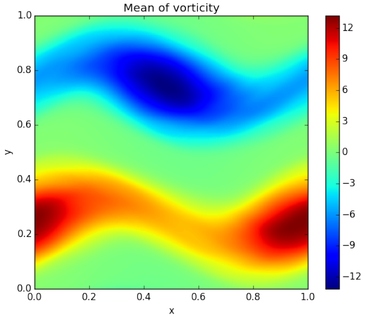
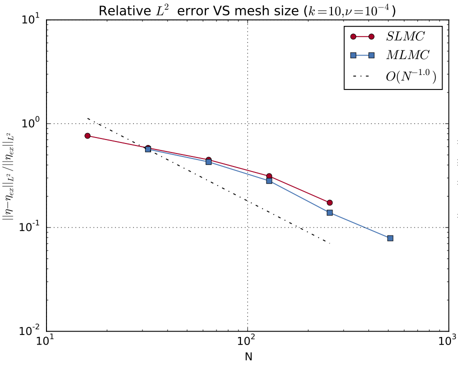
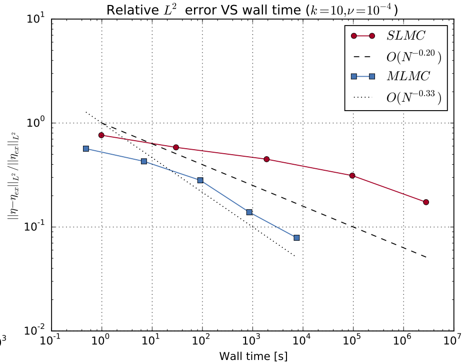


Experiment 2: (smooth) shear layer II, error plots





Conclusion

1. we have a notion of stat. sol. for the **vorticity formulation** of NSE
2. we have a convergent **numerical algorithm** for individual solutions
3. we can compute **approximations of statistical solutions**
4. MLMC accelerates SLMC

Future

1. extend to 3D, different boundary types and unstructured grids;
2. what about Euler?
3. what about high order and efficient schemes?

Thanks!

Time for questions...

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