Generation of Multiple Turbulent Flow States for the Simulations With Ensemble Averaging

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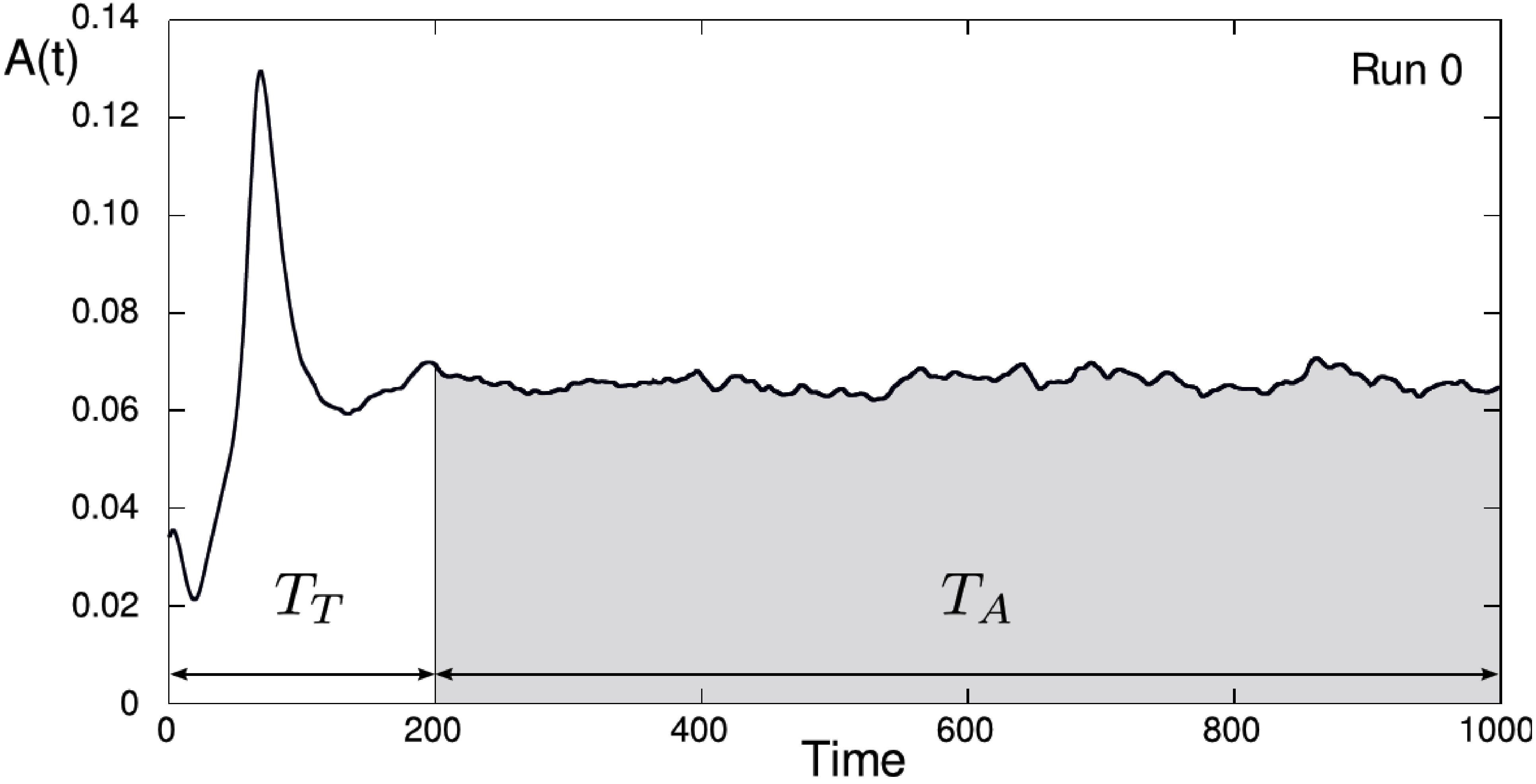
Motivation

High-fidelity turbulent flow simulations assumes:

- ***Eddy-resolving methods (DNS / LES / DES)***
- ***Huge computational grids (10^6-10^{10}-...)***
- ***Long time integration to collect turbulent statistics (10^4-... time steps)***

Typical DNS / LES simulation

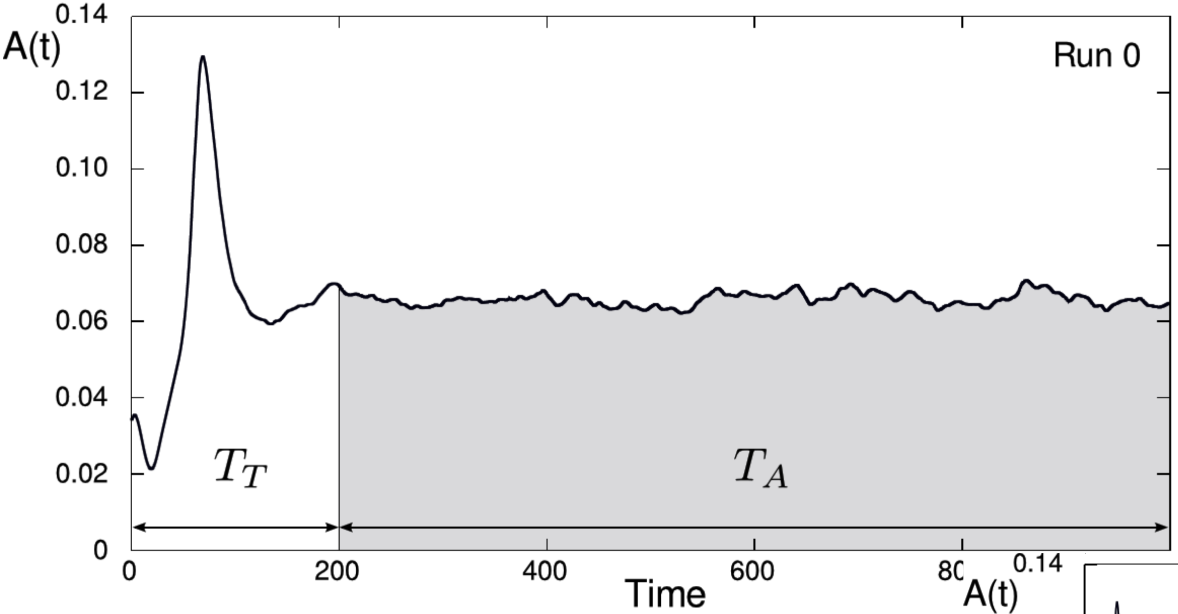


Overall simulation: $T = T_T + T_A$

***Evolution of integral velocity perturbations amplitude in a straight pipe**

Parallelization in time

Simulation with two different initial states

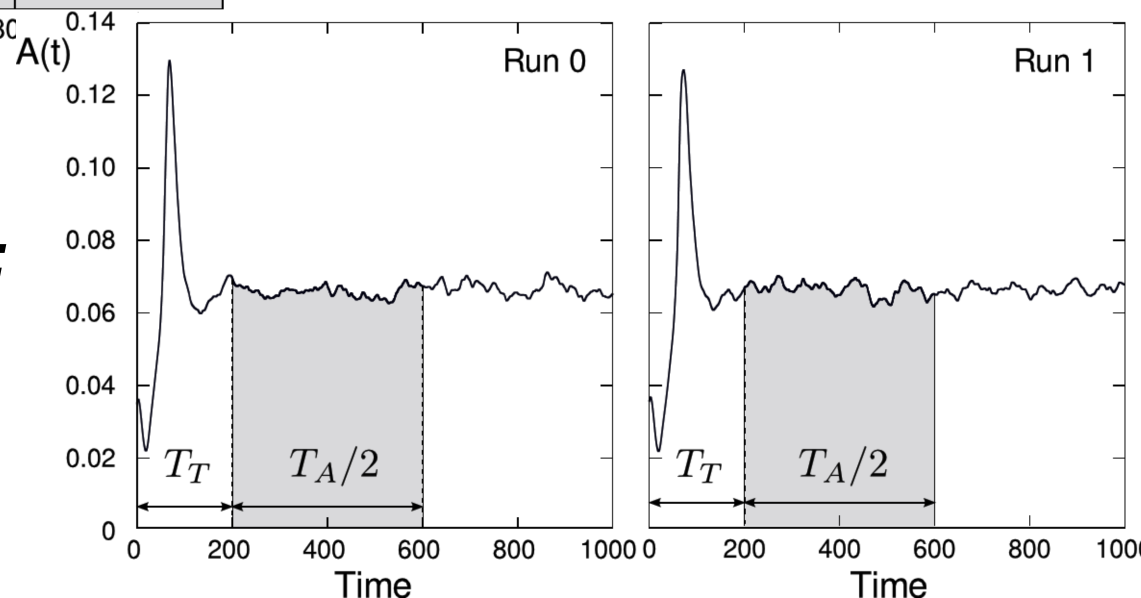


Overall time:

$$T_{total} = 2T_T + T_A$$

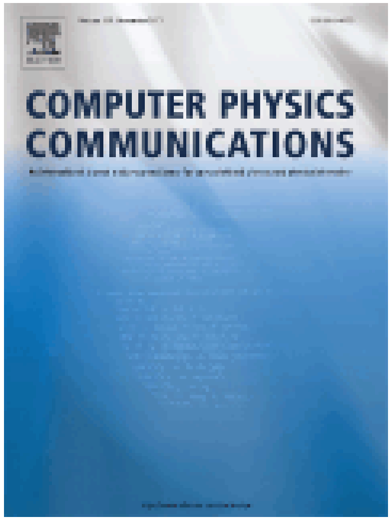
Simulation time per each run:

$$T_1 = T_T + T_A/2$$



Ensemble averaging (1)

V. Makarashvili, E. Merzari, A. Obabko, A. Siegel, P. Fischer. **A performance analysis of ensemble averaging for high fidelity turbulence simulations at the strong scaling limit** // *Computer Physics Communications*, vol. 219, 2017, p. 236-245



- ***m** independent runs*
- *Speedup due to increase of computational resources*

Time integration (1)

Typical methods for modelling incompressible turbulent flows with eddy-resolving models:

- ***High-order Runge-Kutta time integration schemes (one of substeps):***

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\left(\mathbf{u}^n \cdot \nabla\right)\mathbf{u}^n + \frac{1}{Re}\nabla^2\mathbf{u}^n$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla p^{n+1}$$

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t}\nabla \cdot \mathbf{u}^*$$

- ***Krylov subspace & Multigrid methods for solving pressure Poisson equations***

Time integration (2)

Typical methods for modelling incompressible turbulent flows with eddy-resolving models:

- ***High-order Runge-Kutta time integration schemes (one of substeps):***

$$\frac{\mathbf{U}^* - \mathbf{U}^n}{\Delta t} = -\left(\mathbf{U}^n \cdot \nabla\right)\mathbf{U}^n + \frac{1}{Re}\nabla^2 \mathbf{U}^n$$

$$\mathbf{U}^{n+1} = \mathbf{U}^* - \Delta t \nabla P^{n+1}$$

$$\nabla^2 P^{n+1} = \frac{1}{\Delta t}\nabla \cdot \mathbf{U}^*$$

- ***«Generalized» velocity & pressure:***

$$\mathbf{U} = \{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_m\} \qquad P = \{p_1, p_2, \ldots, p_m\}$$

- ***Pressure Poisson equation with multiple right-hand sides***

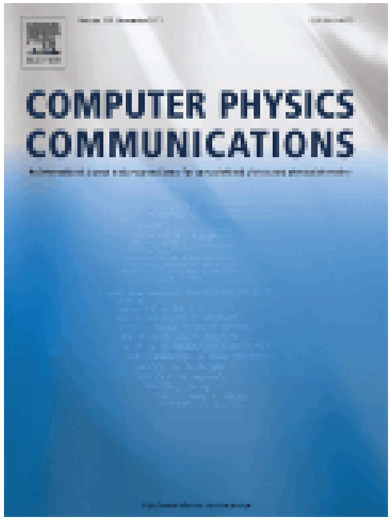
PPE with multiple RHSs

Basic aspects for Krylov subspace & Multigrid methods:

- ***Sparse matrix storage formats (e.g., CSR)***
- ***Operations with vectors (linear operations, scalar products)***
  - *memory bound (e.g., STREAM benchmark)*
- ***Sparse Matrix-Vector multiplications (SpMV)***
  - *memory bound*

- ***Generalized SpMV with multiple RHSs allows to significantly increase the performance due to increase of the computational intensity (flop per byte ratio)***

Ensemble averaging (2)



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- ***m** independent runs*
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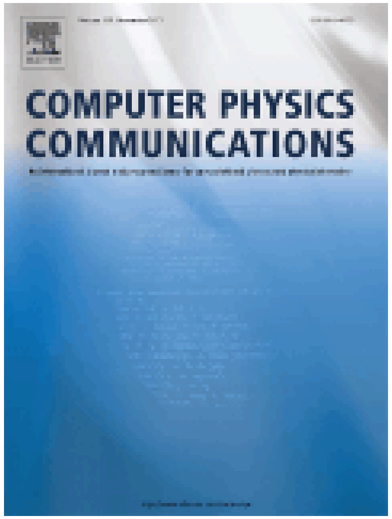


B. Krasnopolsky. **An approach for accelerating incompressible turbulent flow simulations based on simultaneous modelling of multiple ensembles** // *Computer Physics Communications*, vol. 229, 2018, p. 8-19

- *Simultaneous modelling of **m** states in a single run*
- *Speedup due to memory traffic reduction when solving pressure Poisson equation*

Simulation speedup theoretical estimates (1)

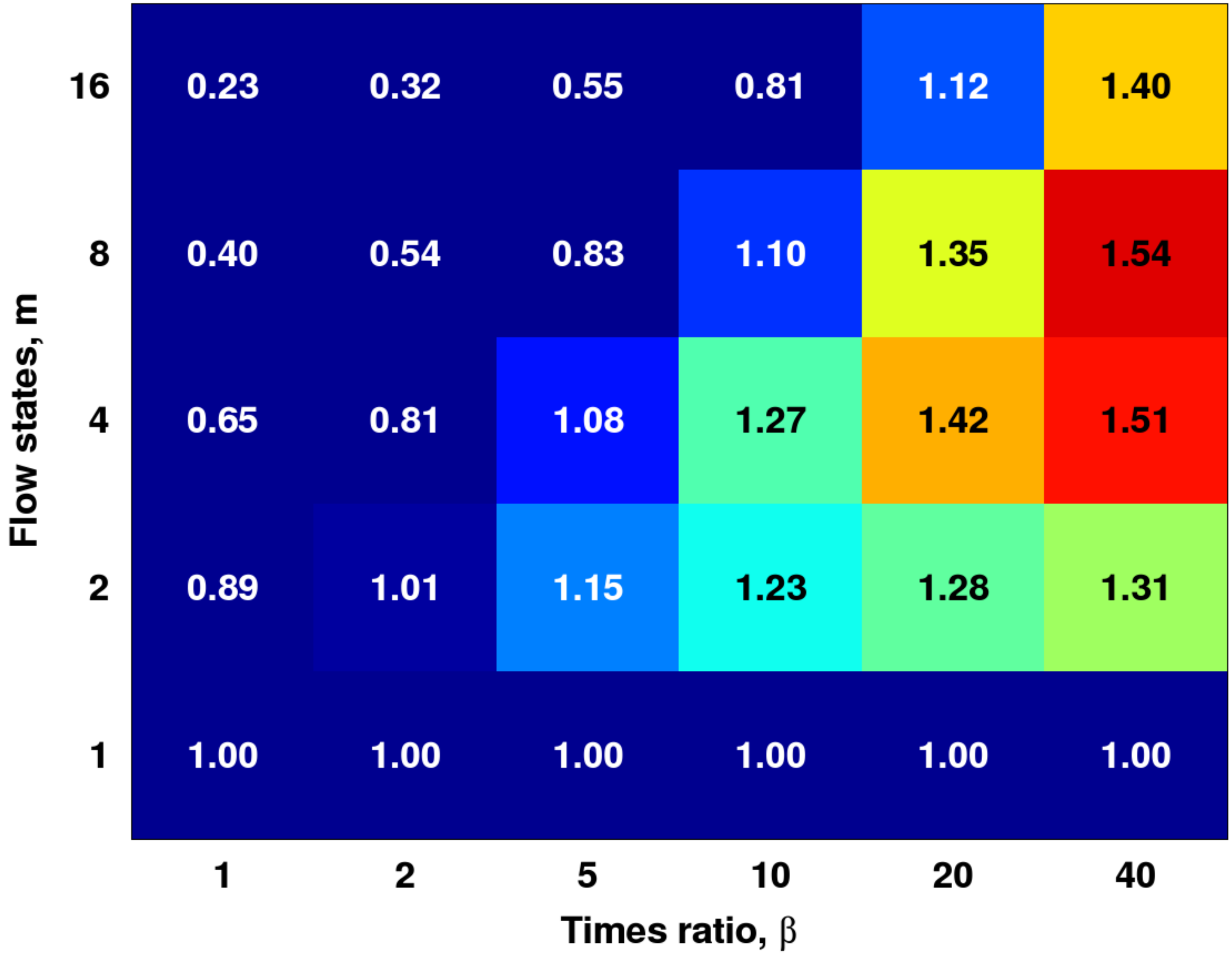
$$P_m = \frac{1+\beta}{m+\beta}\frac{5m}{5m-3\theta(m-1)}$$

Three parameters:

$\beta = T_A/T_T$	***Time intervals ratio; determined by the problem statement***
θ	***SLAE solver time ratio; determined by the choice of the numerical methods used***
m	***Number of simultaneously modelled flow states***

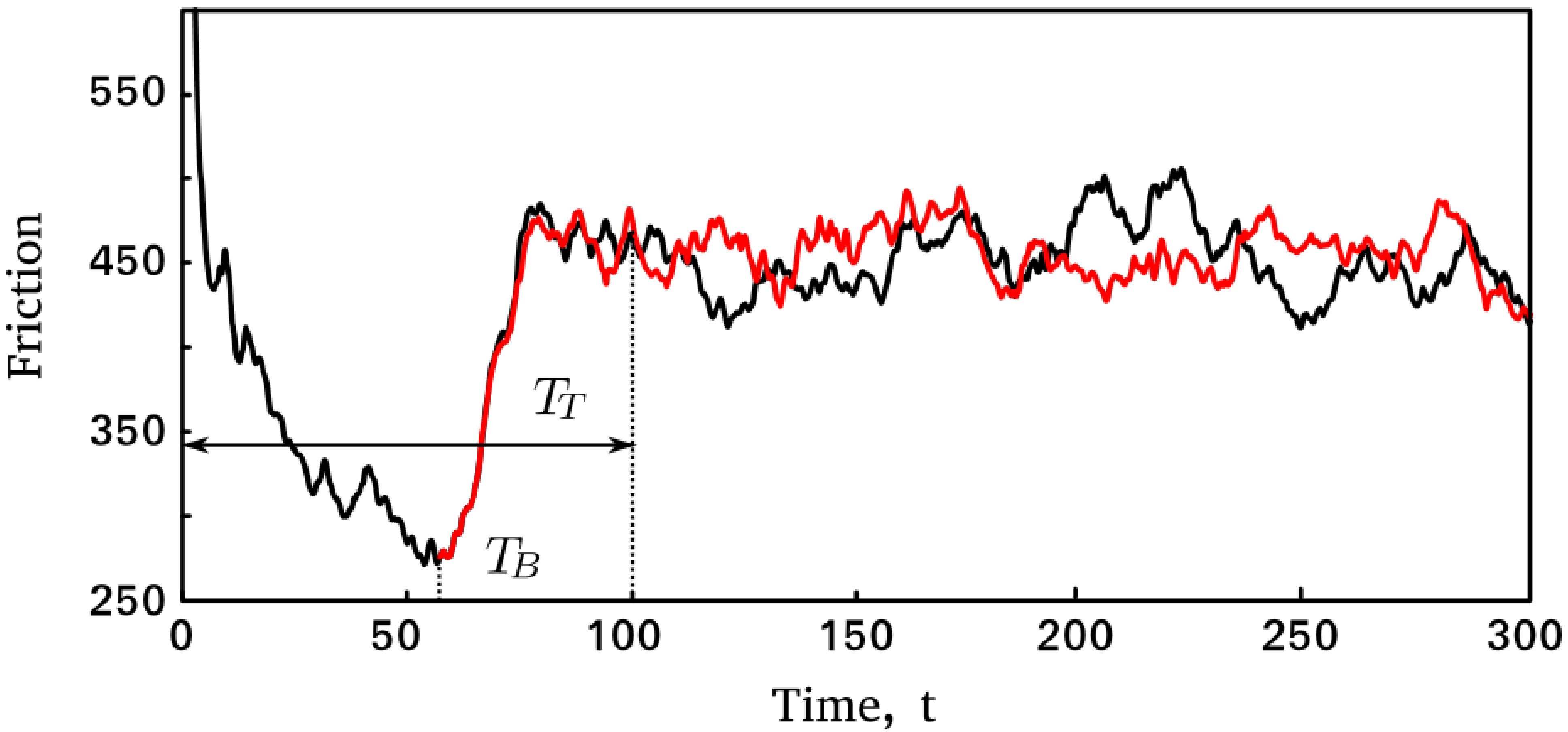
Simulation speedup theoretical estimates (2)

Simulation speedup as a function of a number of flow states:



$$\theta = 0.85$$

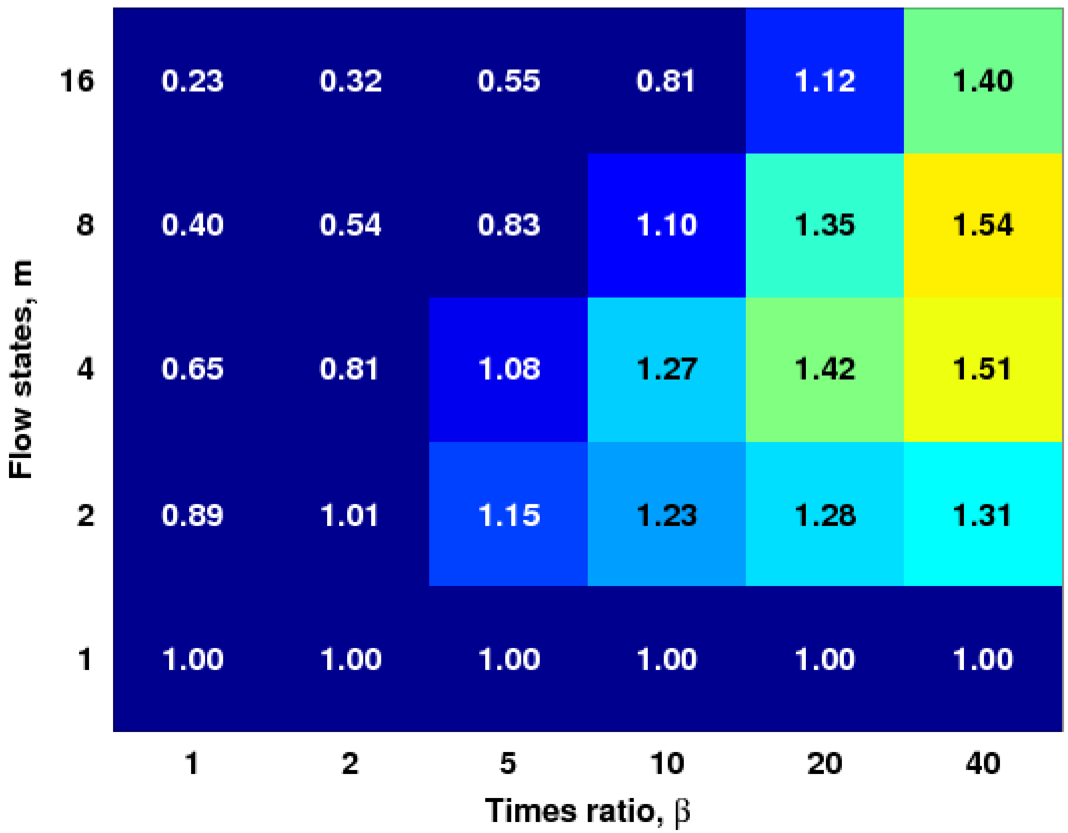
Generation of multiple flow states

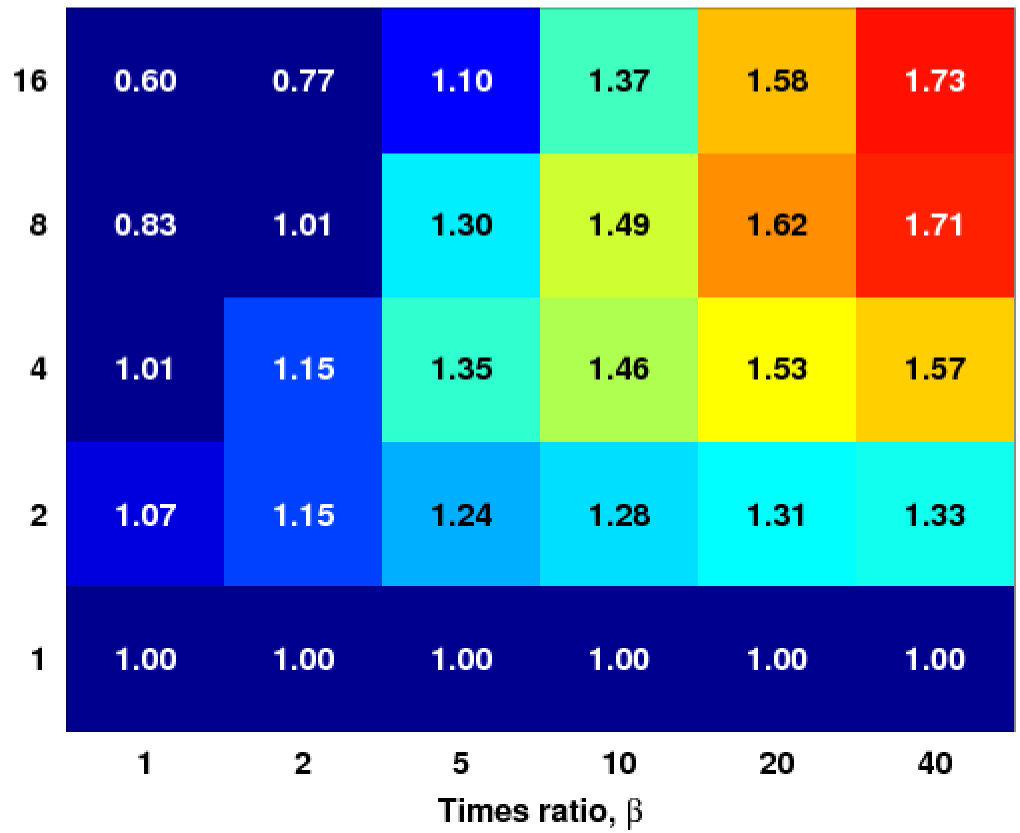


Introducing perturbations at the transition stage (T_B):

$$T_T - T_B \gtrsim T_{corr}$$

Influence on the simulation speedup





$$T_B = 0$$

$$T_B / T_T = 0.75$$

Computational codes

Software:

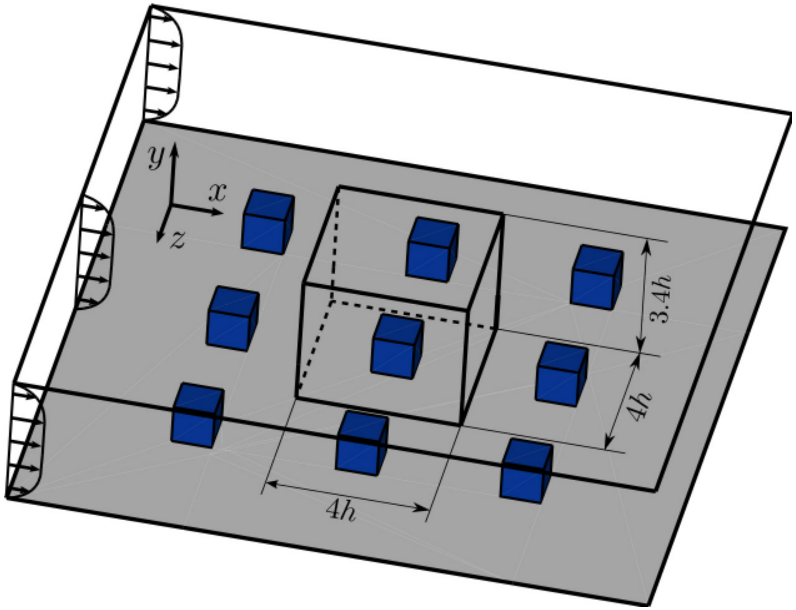
- ***Linear solver for SLAEs with multiple RHSs: BiCGStab + Algebraic Multigrid (hybrid MPI + Posix Shared Memory programming model)***
- ***In-house code for Direct Numerical Simulation of turbulent flows, allowing simultaneous modelling of multiple flow states****

** N. Nikitin. Finite-difference method for incompressible Navier-Stokes equations in arbitrary orthogonal curvilinear coordinates // JCP, 217(2), 759-781, 2006.*

Test problem

Flow in a channel with a matrix of wall-mounted cubes:

- ***No-slip bc at the channel and cube walls***
- ***Periodic bc at lateral faces***
- ***Reynolds number:*** $\mathrm{Re}_b = \dfrac{U_b h}{\nu} = 3854$
- ***Integration intervals: T_T = 100; T_A = 2000***



	Grid 1	Grid 2	Grid 3
Grid size	144 x 112 x 144	240 x 168 x 240	360 x 252 x 360
Cube	52 x 38 x 52	100 x 74 x 100	150 x 120 x 150
h_x, h_z	$0.0065h - 0.054h$	$0.0031h - 0.038h$	$0.0024h - 0.023h$
h_y	$0.0054h - 0.07h$	$0.003h - 0.044h$	$0.0023h - 0.03h$
Overall size	2.32 M	9.68 M	32.7 M

Simulation results

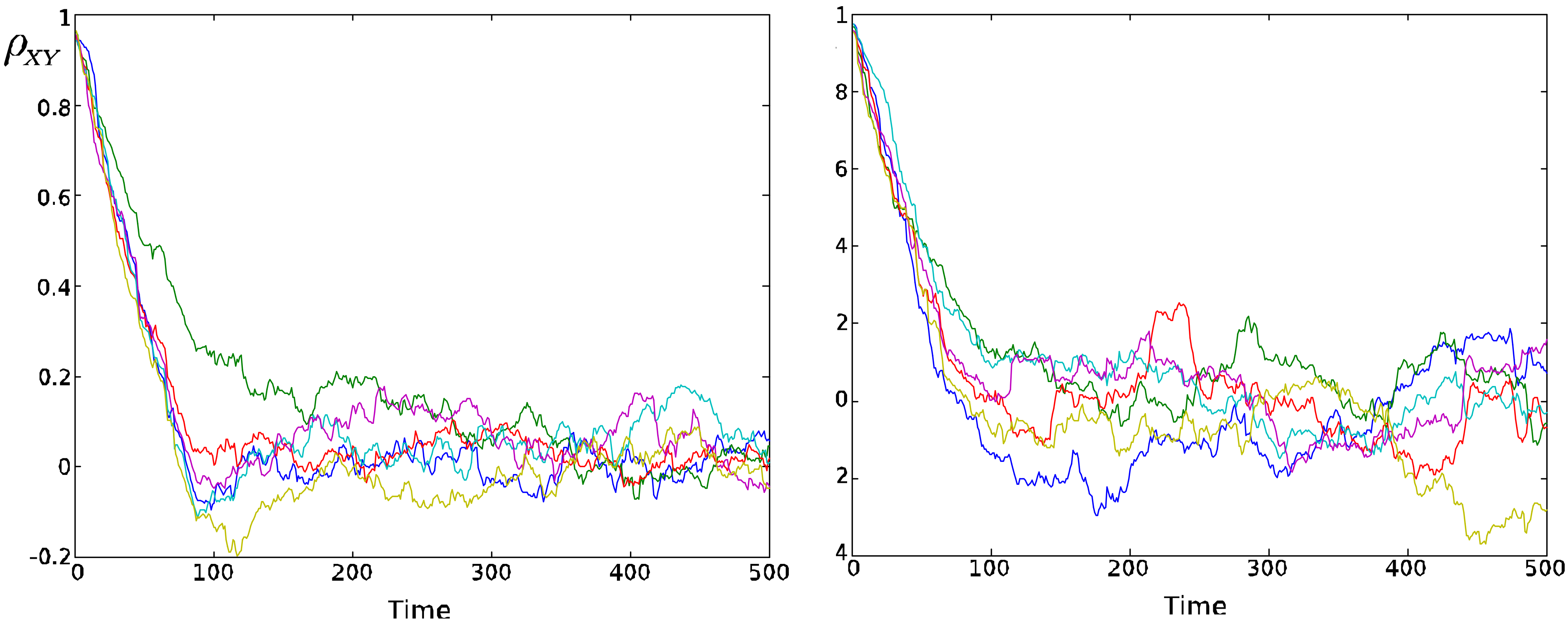
Test case: Grid 1, 2.32 M cells

- ***32 nodes, "Lomonosov-2" (448 cores)***

Flow states, m	T_B / T_T	CPU time, min	Expected speedup	Actual speedup
1	-	1088	-	-
4	0	790	1.42	1.38
4	0.77	729	1.53	1.49
8	0.77	695	1.63	1.57

Cross-correlation for different flow states

Cross-correlation of the time series for the longitudinal velocity components of 4 flow states



Conclusion

- ***The methodology of generation multiple uncorrelated turbulent flow states based on introducing perturbations during the transition stage has been investigated***
- ***The performance gain theoretical estimate has been extended to cover the simulation scenario of interest***
- ***Actual simulation speedup agrees with the proposed estimates***
- ***The proposed methodology:***
  - ***Extends the range of applicability for the ensemble averaging approach***
  - ***Provides additional 20% simulation speedup***

List of publications

- *B. Krasnopolsky.* **An approach for accelerating incompressible turbulent flow simulations based on simultaneous modelling of multiple ensembles** // *Computer Physics Communications*, v. 229, 2018, p. 8–19.
- *B. Krasnopolsky.* **Optimal strategy for modelling turbulent flows with ensemble averaging on high performance computing systems** // *Lobachevskii Journal of Mathematics*. v. 39 (4), 2018, p. 533–542.
- *B. Krasnopolsky.* **Generation of multiple turbulent flow states for the simulations with ensemble averaging** // *Supercomputing Frontiers and Innovations*, v. 5 (2), 2018, p. 55–62.