Parallel CFD 2008

May 19-22, 2008

Lyon, France.

On the extension of the Krylov-Schur-Fourier Decomposition Poisson solver for fully-3D DNS of turbulent flows on supercomputers

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Presentation outline

1. **DNS of turbulent flows**
   - A challenge: flow around fully 3D obstacle
2. **Numerical methods for DNS**
   - Symmetry-preserving discretization of Navier-Stokes equations
   - Pressure-velocity coupling. Poisson equation
   - Poisson solver: extended algorithm for fully-3D geometry
3. **Application: DNS of a surface mounted cube in a channel flow with Re from 2000 to 10000**
4. **Final Conclusions and Current Research**

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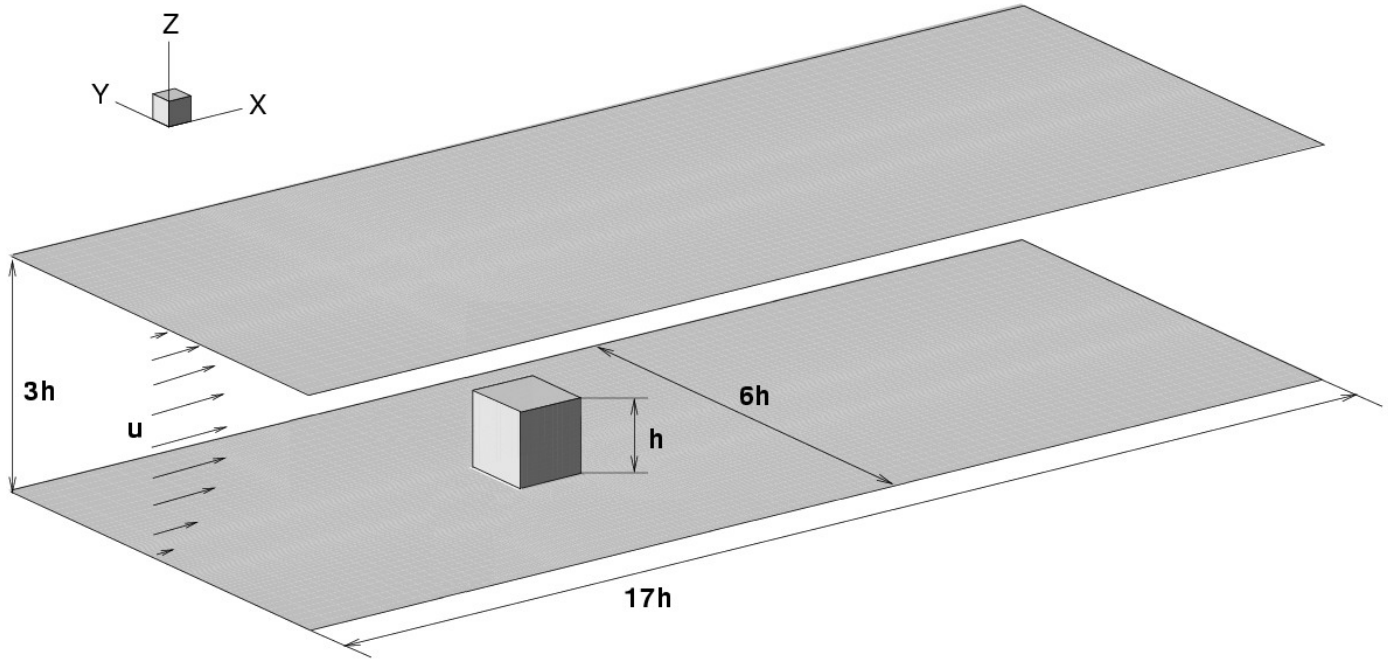
Problem definition: Turbulent flow around a wall-mounted cube

Challenge - mesh sizes 50M - 100M, Re 10000 and more



- **Streamwise x-direction:**
  - Inflow: laminar prolife
  - Outflow: null derivatives
- **Spanwise y-direction: periodic BC/non-slip BC**
- **Wall-normal z-direction: non-slip BC**

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Governing equations

Incompressible Navier-Stokes equations

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\,\boldsymbol{u} - \frac{1}{Re}\Delta \boldsymbol{u} + \nabla p = 0 \qquad\qquad \nabla \cdot \boldsymbol{u} = 0$$

Finite-volume discretization on an **arbitrary staggered mesh** can be written by

$$\Omega_s \frac{d\boldsymbol{u}_s}{dt} + \mathsf{C}\,(\boldsymbol{u}_s)\,\boldsymbol{u}_s + \mathsf{D}\boldsymbol{u}_s + \Omega_s \mathsf{G}\boldsymbol{p}_c = \boldsymbol{0}_s \qquad\qquad \mathsf{M}\boldsymbol{u}_s = \boldsymbol{0}_c$$

- Ω_s is a diagonal matrix with the sizes of **control volumes**.
- The matrices $\mathsf{C}\,(\boldsymbol{u}_s)$ and D are the **convective** and **diffusive** operators, respectively.
- G represents the discrete **gradient** operator
- M is the integral of the **divergence** operator

High-accurate DNS numerical solutions over the past decades have evidenced that these equations form an excellent mathematical model for turbulent flow.

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Symmetry-preserving discretization

Idea behind: **mimicking the crucial symmetry properties of the underlying differential operators**.

$$\Omega_s \frac{d\boldsymbol{u}_s}{dt} + \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{u}_s + \mathsf{D}\boldsymbol{u}_s + \Omega_s \mathsf{G}\boldsymbol{p}_c = \boldsymbol{0}_s$$

$$\mathsf{M}\boldsymbol{u}_s = \boldsymbol{0}_c$$

$\Longrightarrow$ It can be shown that the **convective matrix** $\mathsf{C}\left(\boldsymbol{u}_s\right)$ has to be **skew-symmetric**,

$$\mathsf{C}\left(\boldsymbol{u}_s\right) + \mathsf{C}^*\left(\boldsymbol{u}_s\right) = 0$$

and the discrete **gradient operator** G has to be exactly equal to...

$$\mathsf{G} = -\Omega_s^{-1}\mathsf{M}^*$$

Pressure-velocity coupling (1/3)

Semi-discrete momentum equation is expressed as

$$\frac{\partial \boldsymbol{u}_s}{\partial t} = \boldsymbol{R}\left(\boldsymbol{u}_s\right) - \mathsf{G}\boldsymbol{p}_c$$

where $\boldsymbol{R}\left(\boldsymbol{u}_s\right) = -\mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{u}_s - \mathsf{D}\boldsymbol{u}_s + \boldsymbol{f}_s$

- **Time discretization:**
  - Central difference is used for the time derivative term
  - Fully explicit second-order Adams-Bashforth scheme for $\boldsymbol{R}\left(\boldsymbol{u}_s\right)$
  - Implicit first-order Euler scheme for pressure-gradient term and mass-conservation equation
- **Spatial discretization:** symmetry-preserving discretization.

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Pressure-velocity coupling (2/3)

Time-discrete system to be solved:

$$\begin{aligned} \frac{\boldsymbol{u}_s^{n+1} - \boldsymbol{u}_s^n}{\Delta t} &= \frac{3}{2}\boldsymbol{R}^n - \frac{1}{2}\boldsymbol{R}^{n-1} - \mathsf{G}\boldsymbol{p}_c^{n+1} \\ \mathsf{M}\boldsymbol{u}_s^{n+1} &= \mathbf{0}_c \end{aligned}$$

Predictor velocity is defined as $\boldsymbol{u}_s^p = \boldsymbol{u}_s^n + \Delta t \left(\frac{3}{2}\boldsymbol{R}^n - \frac{1}{2}\boldsymbol{R}^{n-1} \right)$

$\Longrightarrow$ Then, the unknown velocity is $\boldsymbol{u}_s^{n+1} = \boldsymbol{u}_s^p - \mathsf{G}\tilde{\boldsymbol{p}}_c$

To evaluate $\tilde{\boldsymbol{p}}_c = \Delta t \boldsymbol{p}_c^{n+1}$, **mass conservation** equation **is imposed**

$$\mathsf{M}\boldsymbol{u}_s^{n+1} = \mathsf{M}\boldsymbol{u}_s^p - \mathsf{MG}\tilde{\boldsymbol{p}}_c = \mathbf{0}_c$$

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Pressure-velocity coupling (3/3)

Poisson equation

Recalling that $\mathsf{G} = -\Omega_s^{-1}\mathsf{M}^*$, this leads to the following **Poisson equation**

$$\underbrace{-\mathsf{M}\Omega_s^{-1}\mathsf{M}^*}_{\mathsf{L}}\tilde{\boldsymbol{p}}_c = \mathsf{L}\tilde{\boldsymbol{p}}_c = \mathsf{M}\boldsymbol{u}_s^p$$

that must be solved to evaluate $\tilde{\boldsymbol{p}}_c$ and then $\boldsymbol{u}_s^{n+1}$

- Note that the **Laplacian operator** is approximated by the matrix

  $$\mathsf{L} = -\mathsf{M}\Omega_s^{-1}\mathsf{M}^*$$

  which is **symmetric** and **negative-definite**, **like the continuous Laplacian operator**.

- This approach is similar in all the segregated formulations for incompressible flows (DNS/LES).

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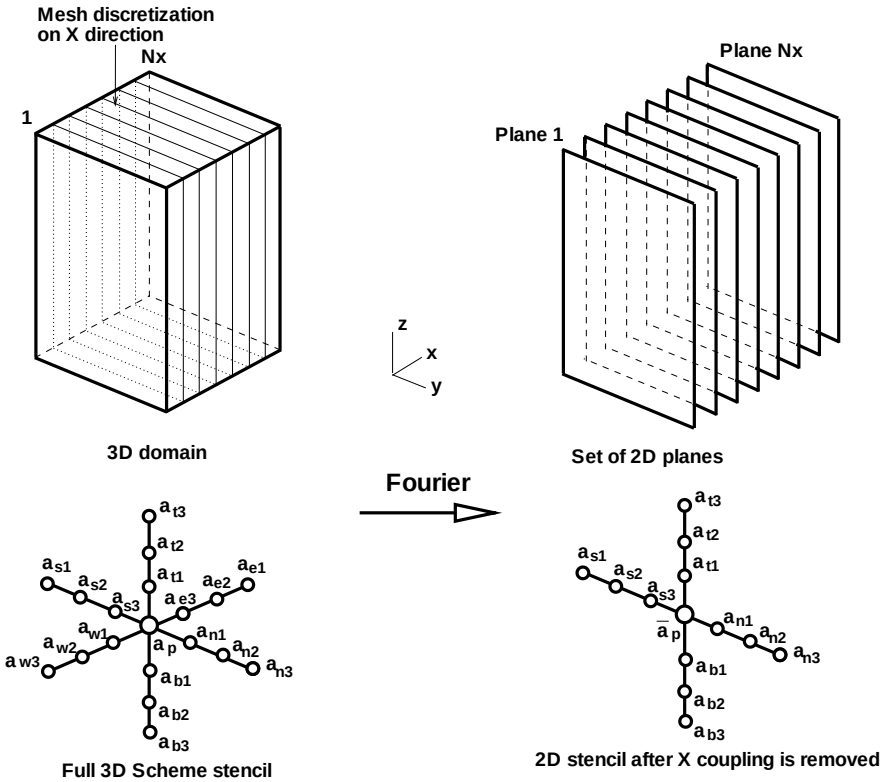
Krylov-Schur-Fourier Decomposition: scalable algorithm



- **KSFD** is a combination of a **FFT-based** method and **Krylov** method of Conjugated Gradients preconditioned with **Direct Schur** method:
  - Fourier diagonalization is applied to reduce the 3D problem in a set of 2D problems.
  - Each 2D problem is solved with a direct DSD method or **CG** iterative method.

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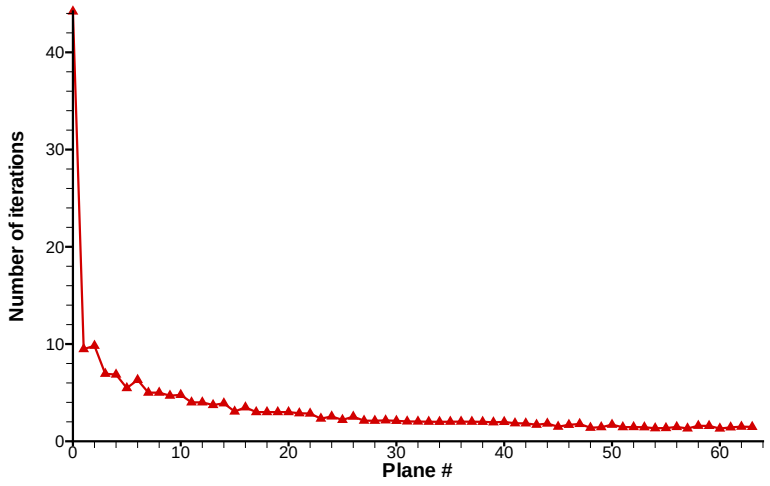
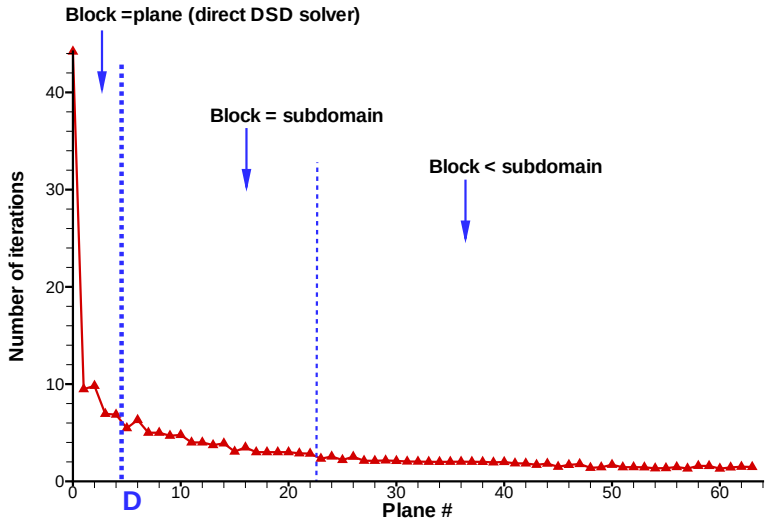
Flexible KSFD configuration

FFT provides a set of 2D independent systems with significantly different condition numbers

- Planes with number $1 \leq i \leq D$ are solved directly by **DSD** method
- Planes with number $D < i \leq N_x$ are solved using CG with local **LU** preconditioner
- **Small** D - to perform well with big meshes on a supercomputer using hundreds of CPU
- **Big** D - to perform well with smaller meshes on a loosely-coupled PC cluster



Typical distribution of the number of iterations

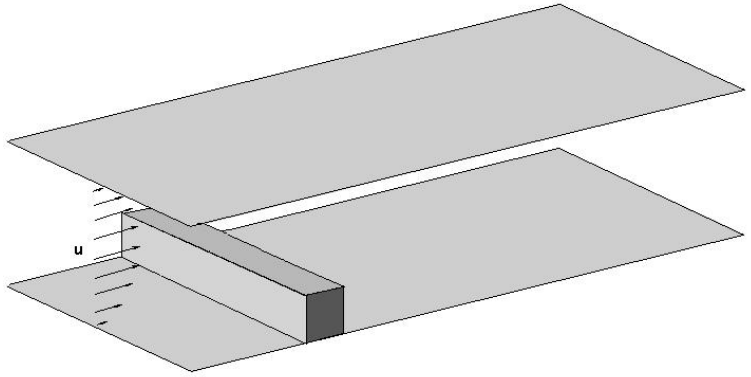


KSFD limitations

the use of FFT implies the following restrictions:

- Mesh must be uniform in the direction where FFT is applied.
- Obstacles geometry is restricted to be 2D extruded on the FFT direction.

This kind of geometry with restrictions will be denoted as "limited-3D"geometry as it is in fact an extrusion of 2D geometry with a constant mesh step.



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Extension to fully-3D geometry

Extension is based on approximation of fully-3D case by means of some limited-3D case which can be solved by KSFD method
while solution of the original fully-3D case is provided by an overlying iterative method.

It can be for example a

- multigrid method (MG) which have limited-3Dcase as a second level
- conjugate gradient method (CG) preconditioined with the limited-3D case

The original fully-3D system to be solved is denoted

$$\mathbf{A}^{3D}\mathbf{x}^{3D} = \mathbf{b}^{3D} \tag{1}$$

and the limited-3D system is

$$\tilde{\mathbf{A}}\mathbf{x} = \mathbf{b} \tag{2}$$

where $\mathbf{A}^{3D}$ and $\tilde{\mathbf{A}}$ are symmetric positive definite matrices.

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MG-KSFD method

MG overlay is considered as it outperformed the CG option in the preliminary convergence tests. So called MG-KSFD method has following algorithm

Algorithm on i-th iteration:

1. Smoother: Obtain approximate solution $\mathbf{x}_i^{3D}$ of (1) using CG with local preconditioner.
2. Calculate residual $\mathbf{r}_i^{3D}$ of system (1).
3. Transform residual to second level $\mathbf{r}_i = \mathbf{Q}\mathbf{r}_i^{3D}$
4. Solve error equation $\tilde{\mathbf{A}}\mathbf{z}_i = \mathbf{r}_i$ on second level using KSFD algorithm.
5. Transform error from second level limited-3D to fully-3D: $\mathbf{z}_i^{3D} = \mathbf{P}\mathbf{z}_i$
6. Correct $\mathbf{x}_{i+1}^{3D} = \mathbf{x}_i^{3D} + \mathbf{z}_i^{3D}$

Here matrixes $\mathbf{Q}$ and $\mathbf{P}$ represent interpolation from first to second level and back respectively.

The two MG levels

First level

- Cube in a flow, non uniform mesh in all directions

Second level

- Uniform mesh on one direction, number of nodes preserved
- No obstacle

In general the idea of the MG-KSFD method is that lower frequencies of the error (most difficult for an iterative solver) are eliminated effectively by the second level solver while higher frequencies are effectively killed by a smoother.

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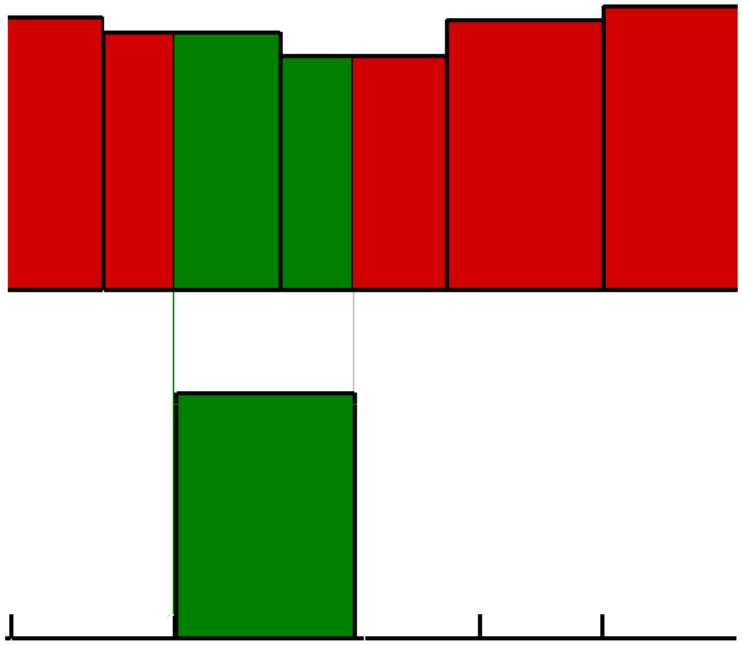
Interpolation to the second level

Volumetric interpolation is used to transit from 1st level to 2nd and back



This interpolation exactly conservative

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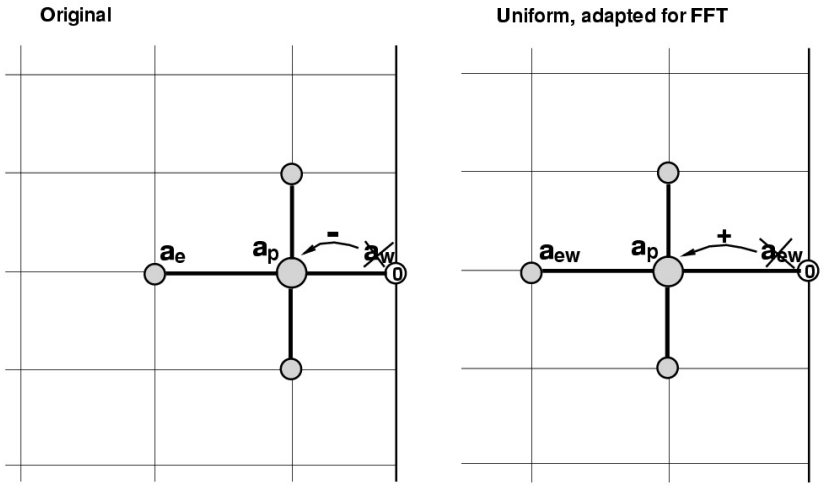
Solution of the second level

For non-slip wall BC transformation of matrix is required to fit FFT compatible form



Second level is solved with KSFD method, high precision is not needed, relative residual decrease 10 times is enough

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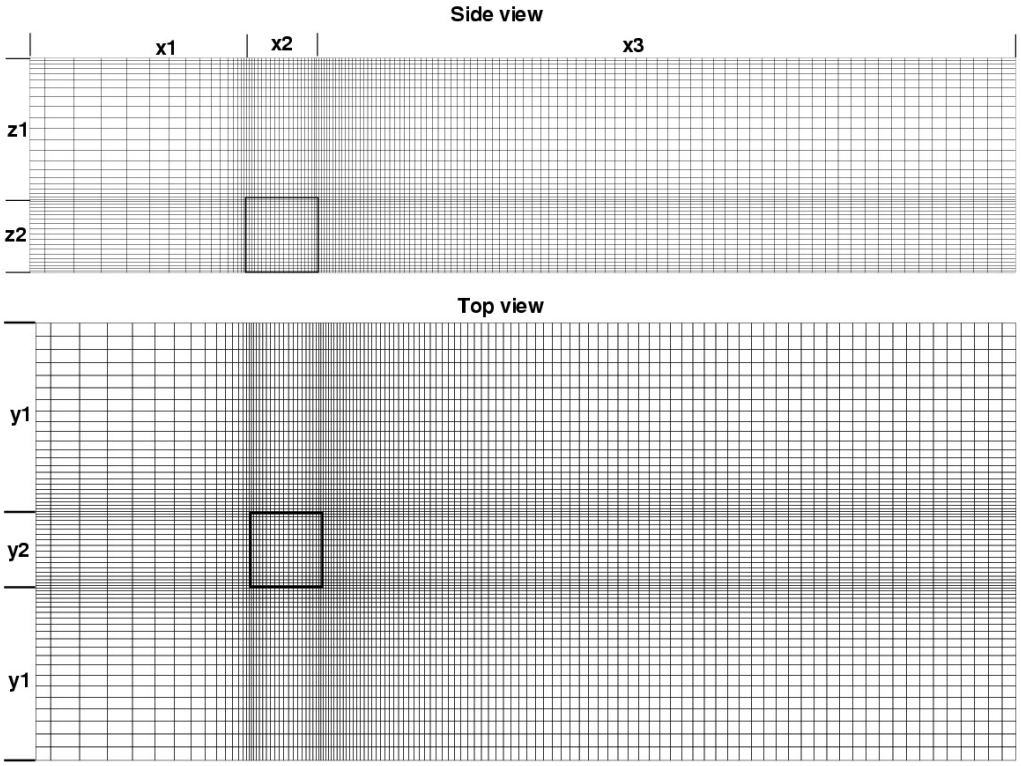
Mesh

Mesh generation is based on concentration function

$$x_i = \frac{L}{2}\left[1 + \frac{\tanh\left(\gamma\left[2(i-1)/N - 1\right]\right)}{\tanh\gamma}\right] \tag{3}$$

L is the length of the fragment, N is the number of nodes in the fragment,
γ is the concentration factor.



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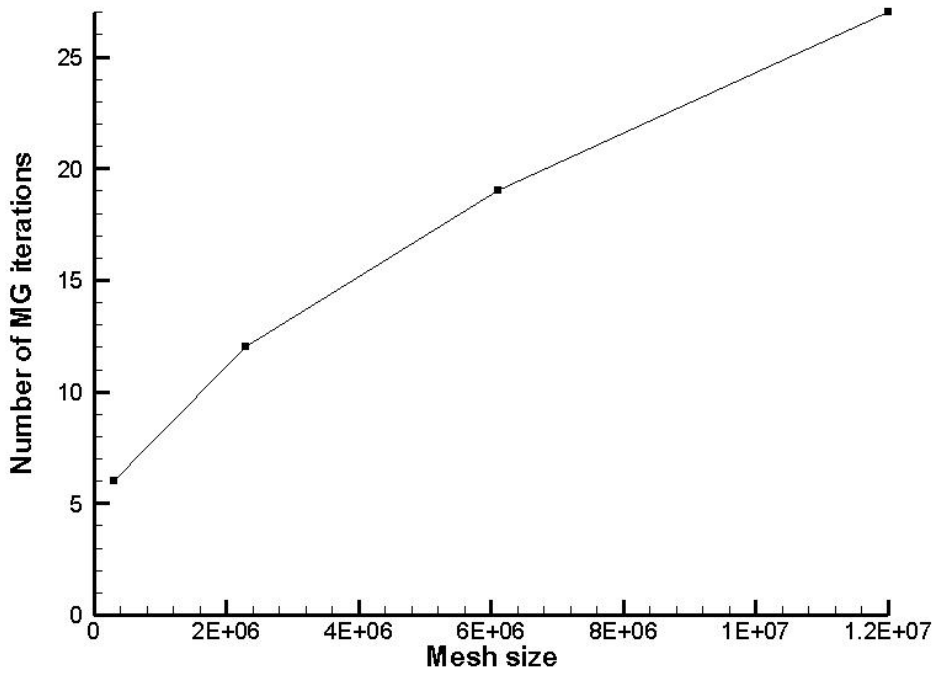
Convergence tests

Test case Re=5000, MG iteration - 15 smoother CG iterations with Jacobi preconditioner and one KSFD solution for the second level



For 25 CG iterations, MG iterations decreased to 13.7 for 12M case

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Expectations

- Convergence and solver performance is not yet what we want.
  Solving cases using 100M mesh within reasonable CPU time is not yet possible...

- But...
  The solver is already robust and can be used for meshes up to 20M - 30M
  and Re > 5000 with fully non-uniform mesh and without any immersed BC etc.

- DNS planned on June will have 20M mesh and Re 5K.

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DNS

A preliminary DNS series of Re 1800 - 2700 and meshes 1M - 2.3M is being performed to find the optimal mesh concentration and to compare with other authors and experimental data