

**JAPAN-RUSSIA WORKSHOP ON SUPERCOMPUTER MODELING, INSTABILITY
AND TURBULENCE IN FLUID DYNAMICS (JR SMIT2015)**
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***Method SMIF for DNS of Incompressible Fluid
Flows.***

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- **Foundation of the problem**
- **Numerical Method SMIF**
- *Monotonous Hybrid Finite-Difference Scheme*
- **Code parallelization**
- **Visualization of the 3D vortex structures**
- *2D-3D transitional flow regimes in the wake of a sphere and a circular cylinder*
- **Conclusion**

Sphere in the stratified fluid

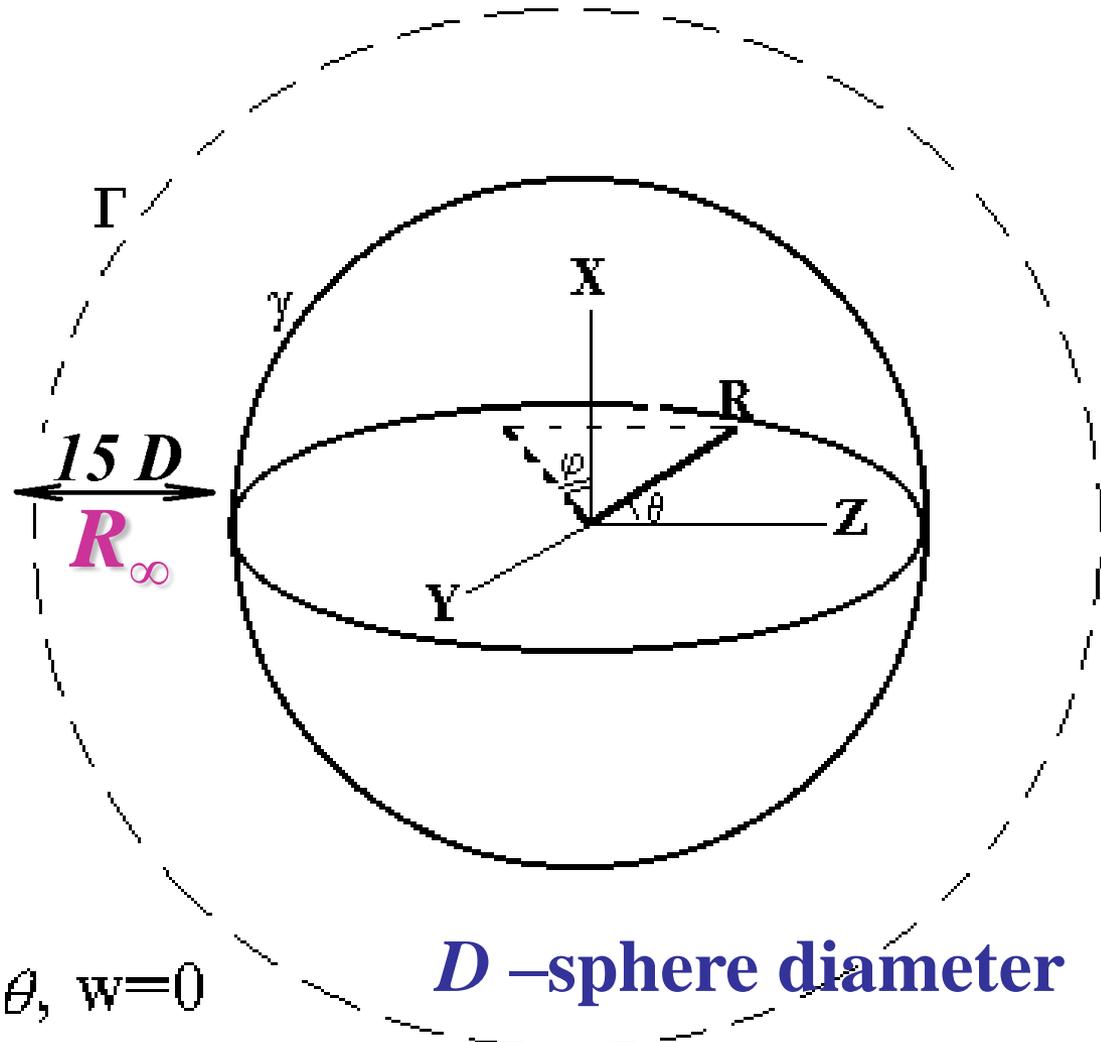
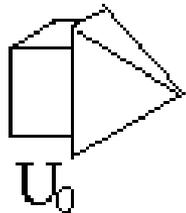
Foundation of the problem



$grid_1=(120 \times 60 \times 120)$

$grid_2=(240 \times 60 \times 120)$

10 points inside of the boundary layer



$$R_\infty = 15 D \div 53 D$$

$$\gamma: u=0, v=0, w=0$$

$$\Gamma: u=U_0 \cos \theta, v=-U_0 \sin \theta, w=0$$

D - sphere diameter

$\vec{g} \downarrow \uparrow \vec{x}$

Navier-Stokes equations in Boussinesq approximation

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \nabla) \vec{v} = -\nabla p + \frac{2}{Re} \Delta \vec{v} + \frac{C}{2Fr^2} s \frac{\vec{g}}{g}$$

approximation

$$Re = U_0 D / \nu$$

$$\nabla \cdot \vec{v} = 0$$

$$Fr = U_0 / ND$$

$$\frac{\partial s}{\partial t} + (\vec{v} \nabla) s = \frac{2}{Sc \cdot Re} \nabla^2 s + \frac{v_x}{2C}$$

$$C = \Lambda / D$$

$$Sc = \nu / k_s$$

$$\rho(x, y, z) = \rho_0 (1 - x / (2C) + s) \quad \text{- density,}$$

p & s – pressure & salinity perturbations, $\mathbf{v} = (v_x, v_y, v_z)$ – velocity vector, U_0 – free-stream velocity,

g – acceleration of gravity,

Λ & N – buoyancy scale and frequency, $\Lambda = g / N^2$

ν – kinematic viscosity, k_s – diffusivity coefficient

Numerical Method *SMIF*

- I
$$\frac{\tilde{\vec{v}} - \vec{v}^n}{\tau} = -(\vec{v}^n \nabla) \vec{v}^n + \frac{2}{\text{Re}} \Delta \vec{v}^n + \frac{C}{2Fr^2} s^n \frac{g}{g}$$
- II
$$\tau \Delta p^{n+1} = \nabla \tilde{\vec{v}} \quad (\text{solved by } \textit{Conjugate Gradients Method})$$
- III
$$\frac{\vec{v}^{n+1} - \tilde{\vec{v}}}{\tau} = -\nabla p^{n+1}$$
- IV
$$\frac{s^{n+1} - s^n}{\tau} = -(\vec{v}^{n+1} \nabla) s^n + \frac{2}{\text{Sc} \cdot \text{Re}} \nabla^2 s^n + \frac{V_x^{n+1}}{2C}$$

Numerical Method

SMIF - *Splitting on physical factors Method for Incompressible Fluids*

O.M. Belotserkovskii, V.A. Gushchin,
V.N. Konshin, V.V. Schennikov

J. Comp. Math. and Math. Phys., 1975, 1987, 1997

The scheme properties:

- second order of accuracy in space
- minimum scheme viscosity and dispersion
- capable for work in wide range of *Re* and *Fr*
- nonoscillating (monotonic)

1D model transfer equation

(How to approximate the convective terms of the equations ?)

$$f_t + uf_x = 0, \quad u = \text{const}$$

Let consider the following two parametric FD scheme:

$$\frac{f_i^{n+1} - f_i^n}{\tau} + u \frac{\tilde{f}_{i+1/2}^n - \tilde{f}_{i-1/2}^n}{h} = 0$$

where

$$\tilde{f}_{i+1/2}^n = \begin{cases} \alpha \begin{pmatrix} f_{i-1}^n \\ f_{i+2}^n \end{pmatrix} + (1 - \alpha - \beta) \begin{pmatrix} f_i^n \\ f_{i+1}^n \end{pmatrix} + \beta \begin{pmatrix} f_{i+1}^n \\ f_i^n \end{pmatrix} & u \geq 0 \\ & u < 0 \end{cases}$$

$$\tilde{f}_{i-1/2}^n = \begin{cases} \alpha \begin{pmatrix} f_{i-2}^n \\ f_{i+1}^n \end{pmatrix} + (1 - \alpha - \beta) \begin{pmatrix} f_{i-1}^n \\ f_i^n \end{pmatrix} + \beta \begin{pmatrix} f_i^n \\ f_{i-1}^n \end{pmatrix} & u \geq 0 \\ & u < 0 \end{cases}$$

Using Taylor's formular in the vicinity of point (i, n) we obtain differential approximation (where $C = |u| \cdot \frac{\tau}{h}$ - Courant number):

$$f_t + uf_x = \frac{Ch^2}{2\tau} \{ \text{sign}u [1 + 2(\alpha - \beta)] - C \} f_{x^2} +$$

	G	CD	UD	MCD	MUD
α	0	0	-0.5	0	-0.5(1-C)
β	0	0.5	0	0.5(1-C)	0
ν_{sch}	$\frac{h}{2} u - \frac{\tau u^2}{2}$	$-\frac{\tau u^2}{2}$	$-\frac{\tau u^2}{2}$	0	0
	$O(h, \tau)$	$O(h^2, \tau)$	$O(h^2, \tau)$	$O(h^2, \tau^2)$	$O(h^2, \tau^2)$

$$0 < C = \frac{\tau|u|}{h} \leq 1, \quad C - \text{Courant number.}$$

$$\alpha = \beta - \frac{1-C}{2}$$

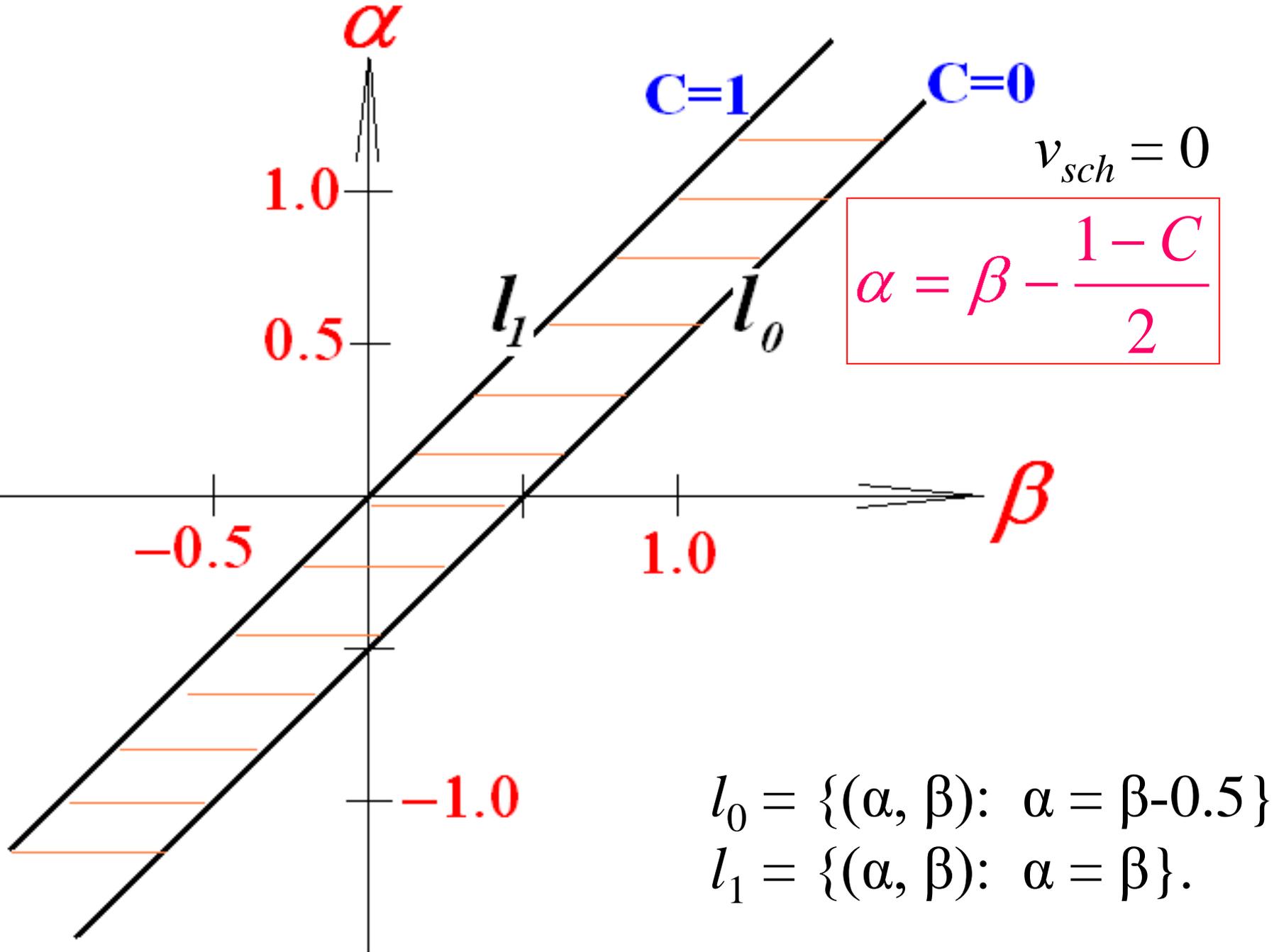
The differential approximation is the following:

$$f_t + u f_x = \frac{Ch^2}{2\tau} [1 + 2(\alpha - \beta) - C] f_{xx} + \frac{Ch^3}{3!\tau} \text{sign} u [1^2 - 6\alpha - 1] f_{xxx} \\ + \frac{Ch^4}{4!\tau} [1 + 14\alpha - 2\beta - C^3] f_{xxxx} + O(\tau^4, h^4).$$

So all the schemes of the second order of accuracy $O(\tau^2, h^2)$ with zero scheme viscosity ($v_{cx} = [1 + 2(\alpha - \beta) - C] \cdot (Ch^2)/(2\tau) = 0$) in (α, β) - plane should be on line

$$\alpha = \beta - \frac{1 - C}{2}.$$

Taking into account that for explicit schemes $0 \leq C \leq 1$, we have that all the schemes of the second order of accuracy with $v_{cx} = 0$ are in the belt between $l_0 = \{(\alpha, \beta): \alpha = \beta - 0.5\}$ и $l_1 = \{(\alpha, \beta): \alpha = \beta\}$ (see fig).



Monotonous Scheme :

The finite-difference scheme is monotonious, if from the following condition:

$$\Delta f_{i+1}^n \equiv f_{i+1}^n - f_i^n \geq 0 \quad (\Delta f_{i+1}^n < 0) \quad \text{for any } i, \text{ we will have that}$$

$$\Delta f_{i+1}^{n+1} \geq 0 \quad (\Delta f_{i+1}^{n+1} < 0) \quad \text{for any } i. \quad (\text{S.K. Godunov-1959})$$

$$\Delta f_{i+1}^{n+1} = \Delta f_{i+1}^n - C \cdot \text{sign } u \left(\tilde{f}_{i+3/2}^n - \tilde{f}_{i+1/2}^n \right) = \Delta f_{i+1}^n - C \cdot \text{sign } u \cdot$$

$$\cdot \left\{ \alpha \begin{pmatrix} \Delta f_i^n \\ \Delta f_{i+3}^n \end{pmatrix} + \left(-\alpha - \beta \right) \begin{pmatrix} \Delta f_{i+1}^n \\ \Delta f_{i+2}^n \end{pmatrix} + \beta \begin{pmatrix} \Delta f_{i+2}^n \\ \Delta f_{i+1}^n \end{pmatrix} - \right.$$

$$\left. - \alpha \begin{pmatrix} \Delta f_{i-1}^n \\ \Delta f_{i+2}^n \end{pmatrix} - \left(-\alpha - \beta \right) \begin{pmatrix} \Delta f_i^n \\ \Delta f_{i+1}^n \end{pmatrix} - \beta \begin{pmatrix} \Delta f_{i+1}^n \\ \Delta f_i^n \end{pmatrix} \right\}$$

$$\Delta f_{i+1}^{n+1} = \Delta f_{i+1} - C \cdot \text{sign } u \left\{ \alpha \left[\begin{pmatrix} \Delta f_i \\ \Delta f_{i+3} \end{pmatrix} - \begin{pmatrix} \Delta f_{i+1} \\ \Delta f_{i+2} \end{pmatrix} - \begin{pmatrix} \Delta f_{i-1} \\ \Delta f_{i+2} \end{pmatrix} + \begin{pmatrix} \Delta f_i \\ \Delta f_{i+1} \end{pmatrix} \right] + \right. \\ \left. + \beta \left[\begin{pmatrix} \Delta f_{i+2} \\ \Delta f_{i+1} \end{pmatrix} - \begin{pmatrix} \Delta f_{i+1} \\ \Delta f_{i+2} \end{pmatrix} - \begin{pmatrix} \Delta f_{i+1} \\ \Delta f_i \end{pmatrix} + \begin{pmatrix} \Delta f_i \\ \Delta f_{i+1} \end{pmatrix} \right] + \begin{pmatrix} \Delta f_{i+1} \\ \Delta f_{i+2} \end{pmatrix} - \begin{pmatrix} \Delta f_i \\ \Delta f_{i+1} \end{pmatrix} \right\}$$

Let $u \geq 0$, then:

$$\Delta f_{i+1}^{n+1} = \Delta f_{i+1} - C \alpha \left[\Delta f_i - \Delta f_{i+1} - \Delta f_{i-1} + \Delta f_i \right] \\ + \beta \left[\Delta f_{i+2} - \Delta f_{i+1} - \Delta f_{i+1} + \Delta f_i \right] + \Delta f_{i+1} - \Delta f_i$$

$$\Delta f_{i+1}^{n+1} = \Delta f_{i+1} - C \left[\beta - \frac{(-C)}{2} \right] \left[\Delta f_{i+1} + 2\Delta f_i - \Delta f_{i-1} \right] + \beta \left[\Delta f_{i+2} - 2\Delta f_{i+1} + \Delta f_i \right] \left[\Delta f_{i+1} - \Delta f_i \right]$$

$$\alpha = \beta - \frac{1-C}{2}$$

$$= -C\beta \Delta f_{i+2} + \left[3C\beta - \frac{C(1-C)}{2} + 1 - C \right] \Delta f_{i+1} + \left[3C\beta + C(1-C) + C \right] \Delta f_i + \left[C\beta - \frac{C(1-C)}{2} \right] \Delta f_{i-1} =$$

$$\Delta^2 f_i^n \equiv \Delta f_i^n - \Delta f_{i-1}^n$$

$$= -C\beta \Delta^2 f_{i+2} + \left[2C\beta - \frac{C(3-C)}{2} + 1 \right] \Delta f_{i+1} + \left[-2C\beta + \frac{C(3-C)}{2} \right] \Delta f_i - \left[C\beta - \frac{C(1-C)}{2} \right] \Delta^2 f_i$$

Let $\Delta f_i^n \geq 0$ for any i , then in order to $\Delta f_i^{n+1} \geq 0$ we demand the positiveness of all items.

Let $\Delta^2 f_{i+2} \geq 0$ and $\Delta^2 f_i \geq 0$, then

$\Delta f_{i+1}^{n+1} \geq 0$, if:

$$\left\{ \begin{array}{l} \beta \leq 0 \\ 2C\beta - C(3-C)/2 + 1 \geq 0 \\ -2C\beta + C(3-C)/2 \geq 0 \\ C\beta - C(1-C)/2 \leq 0 \end{array} \right. \quad \text{or} \quad \left\{ \begin{array}{l} \beta \leq 0 \\ \beta \geq (3-C)/4 - 1/(2C) \\ \beta \leq (3-C)/4 \\ \beta \leq (1-C)/2 \end{array} \right.$$

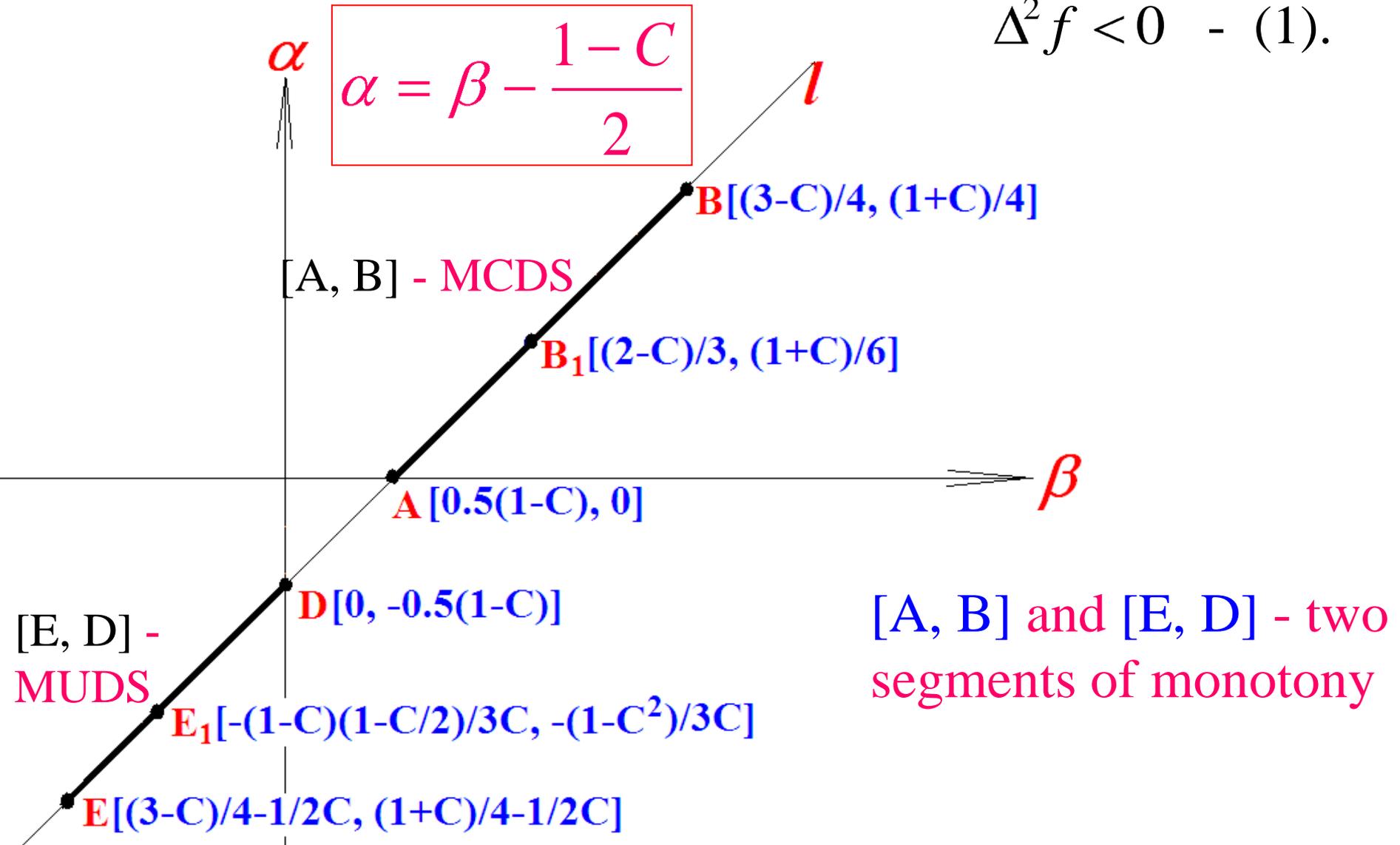
in other words, if $(3-C)/4 - 1/(2C) \leq \beta \leq 0$. (1)

Let $\Delta^2 f_{i+2} < 0$ and $\Delta^2 f_i < 0$, then $\Delta f_{i+1}^{n+1} \geq 0$

, if $(1-C)/2 \leq \beta \leq (3-C)/4$. (2)

Similar we can check, that at $u \geq 0$ from $\Delta f_i^n < 0$ follows that $\Delta f_i^{n+1} < 0$ and at $\Delta^2 f \geq 0$ we have (2), and at $\Delta^2 f < 0$ - (1).

$$\alpha = \beta - \frac{1-C}{2}$$



Similar at $u < 0$ we will have (1) and (2) at corresponding signs of Δf and $\Delta^2 f$.

Let us check that the ranges of monotonicity of MCDS and MUDS have a non-empty intersection.

For $u \geq 0$:

$$\begin{aligned} \Delta f_{i+1}^{n+1} &= -C\beta \Delta f_{i+2} + \left[3C\beta - \frac{C(1-C)}{2} + 1 - C \right] \Delta f_{i+1} + \\ &+ \left[3C\beta + C(1-C) + C \right] \Delta f_i + \left[C\beta - \frac{C(1-C)}{2} \right] \Delta f_{i-1} = \\ &= k_1 \Delta f_{i+2} + k_2 \Delta f_{i+1} + k_3 \Delta f_i + k_4 \Delta f_{i-1}, \end{aligned}$$

AB:

$$k_1 = -C\beta \leq 0, k_2 = 3C\beta + \left(-C \left(1 - \frac{C}{2}\right)\right) \geq 0, k_4 = C \left(\beta - \frac{(1-C)}{2}\right) \geq 0,$$

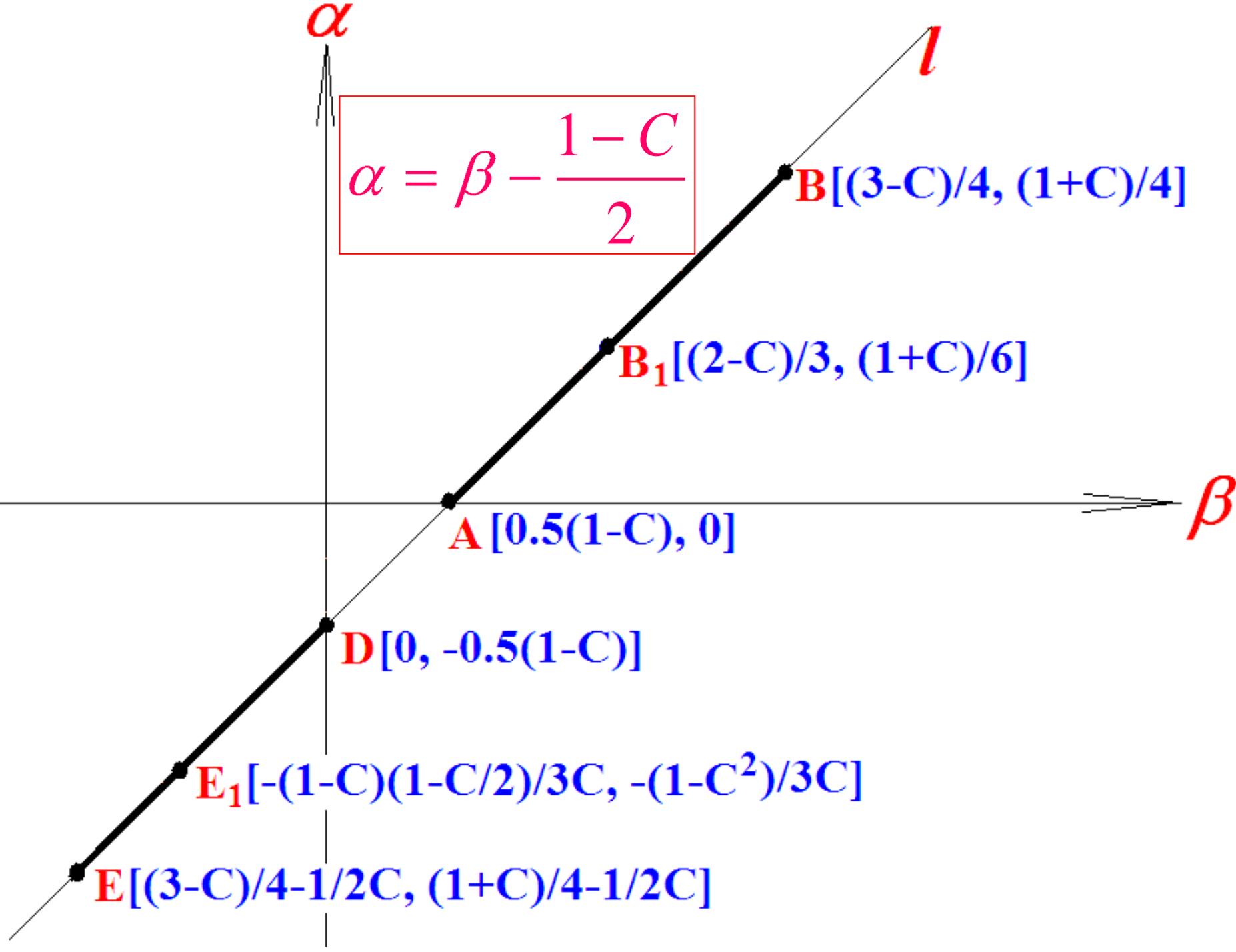
$k_3 = C(2 - C - 3\beta)$ change the sign:

$$\text{at } (1-C)/2 \leq \beta \leq (2-C)/3 \quad k_3 \geq 0.$$

ED:

$k_1 \geq 0, k_3 \geq 0, k_4 \leq 0, k_2 = 3C\beta + (1 - C)(1 - C/2)$ change the sign:
at $-(1 - C)(1 - C/2)/(3C) \leq \beta \leq 0 \quad k_2 \geq 0$

It is possible to conclude that the ranges of monotonicity of MCDS and MUDES from segments B_1B and EE_1 have an empty intersection.



AB₁:

$$k_3 \geq 0, k_4 \geq 0 \text{ and } \Delta f \geq 0$$

$$\text{Let: } -C\beta \Delta f_{i+2} + \left[3C\beta + \left(-C \left(1 - \frac{C}{2} \right) \right) \right] \Delta f_{i+1} \geq 0$$

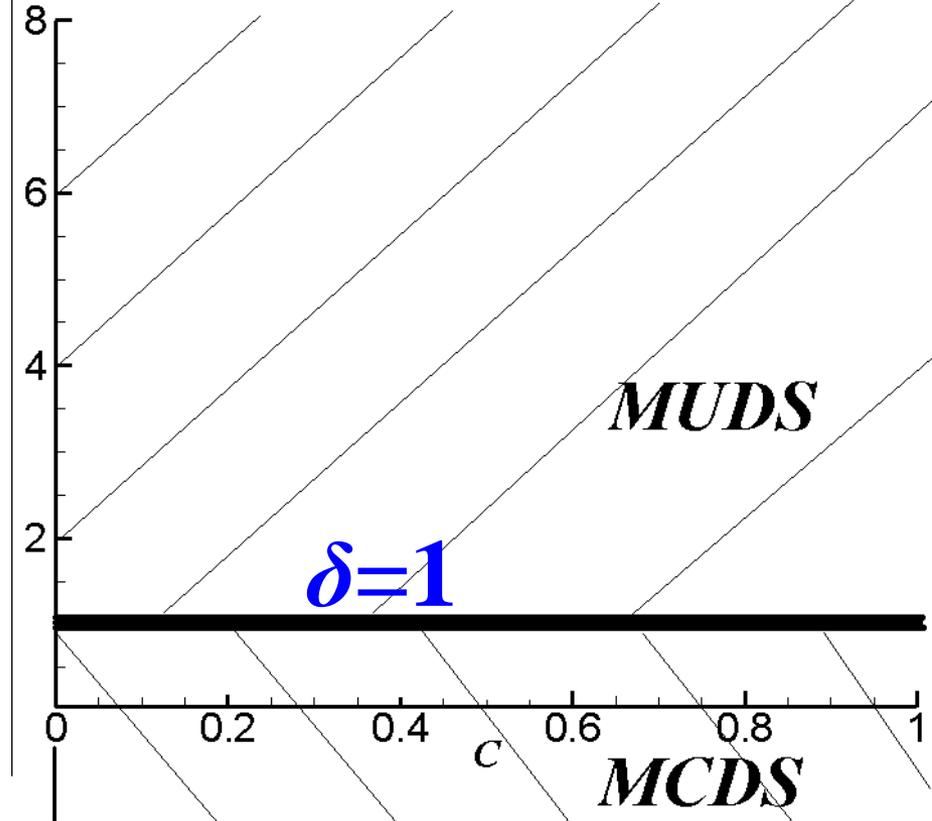
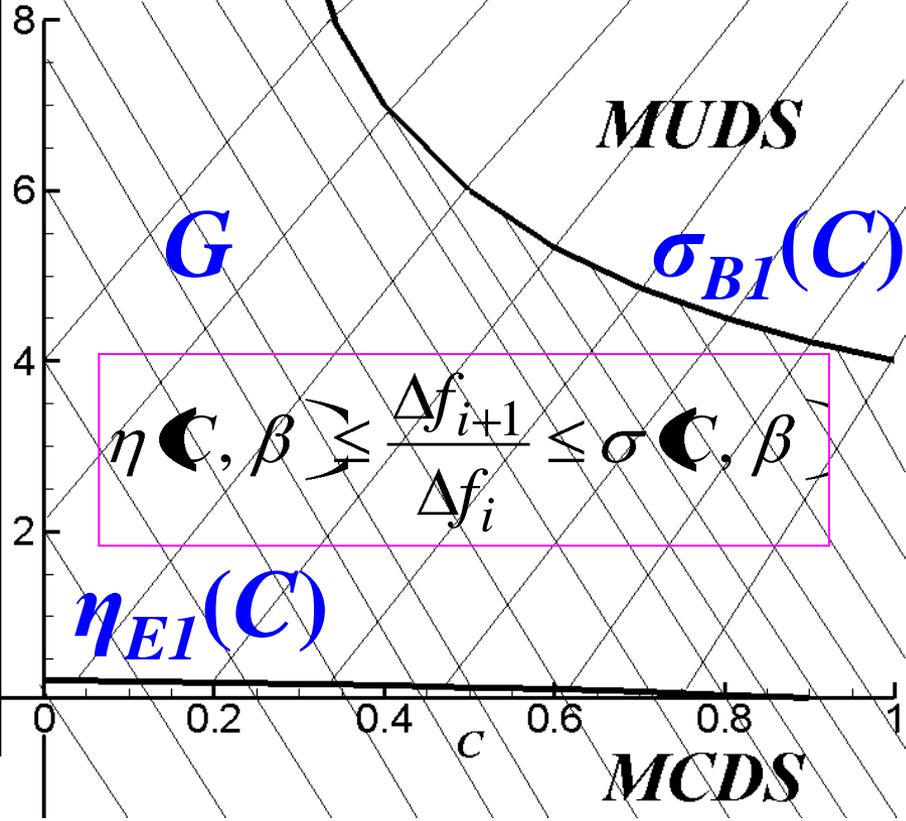
$$\text{or } \frac{\Delta f_{i+2}}{\Delta f_{i+1}} \leq \frac{3C\beta + \left(-C \left(1 - \frac{C}{2} \right) \right)}{C\beta} = \sigma(C, \beta)$$
$$3 \leq \sigma(C, \beta) = 3 + \frac{\left(-C \left(1 - \frac{C}{2} \right) \right)}{2C\beta} < +\infty$$

E₁D:

$$\text{Let: } \left[3C\beta + C(1-C) + C \right] \Delta f_i + \left[C\beta - \frac{C(1-C)}{2} \right] \Delta f_{i-1} \geq 0$$

$$\text{or } \frac{\Delta f_i}{\Delta f_{i-1}} \geq \frac{C\beta - \left(-C \right) C/2}{3C\beta - C(1-C) - C} = \eta(C, \beta)$$

$$0 \leq \eta(C, \beta) = \frac{1}{3} \left[1 + \frac{1}{2} \frac{1+C}{3\beta + C - 2} \right] \leq \frac{1}{3}$$



At:
$$\eta \mathbf{C}, \beta \gtrsim \frac{\Delta f_{i+1}}{\Delta f_i} \leq \sigma \mathbf{C}, \beta$$

The $MCDS$ and $MUDDS$ are monotonious simultaneously.

Let: $\frac{\Delta f_{i+1}}{\Delta f_i} = \delta \in G.$

At $\delta = 1$ the MCDS and MUDS are monotonious at any $C \in [0, 1]$

It means that $\Delta f_{i+1} = \Delta f_i$ or $\Delta^2 f_{i+1} = 0.$

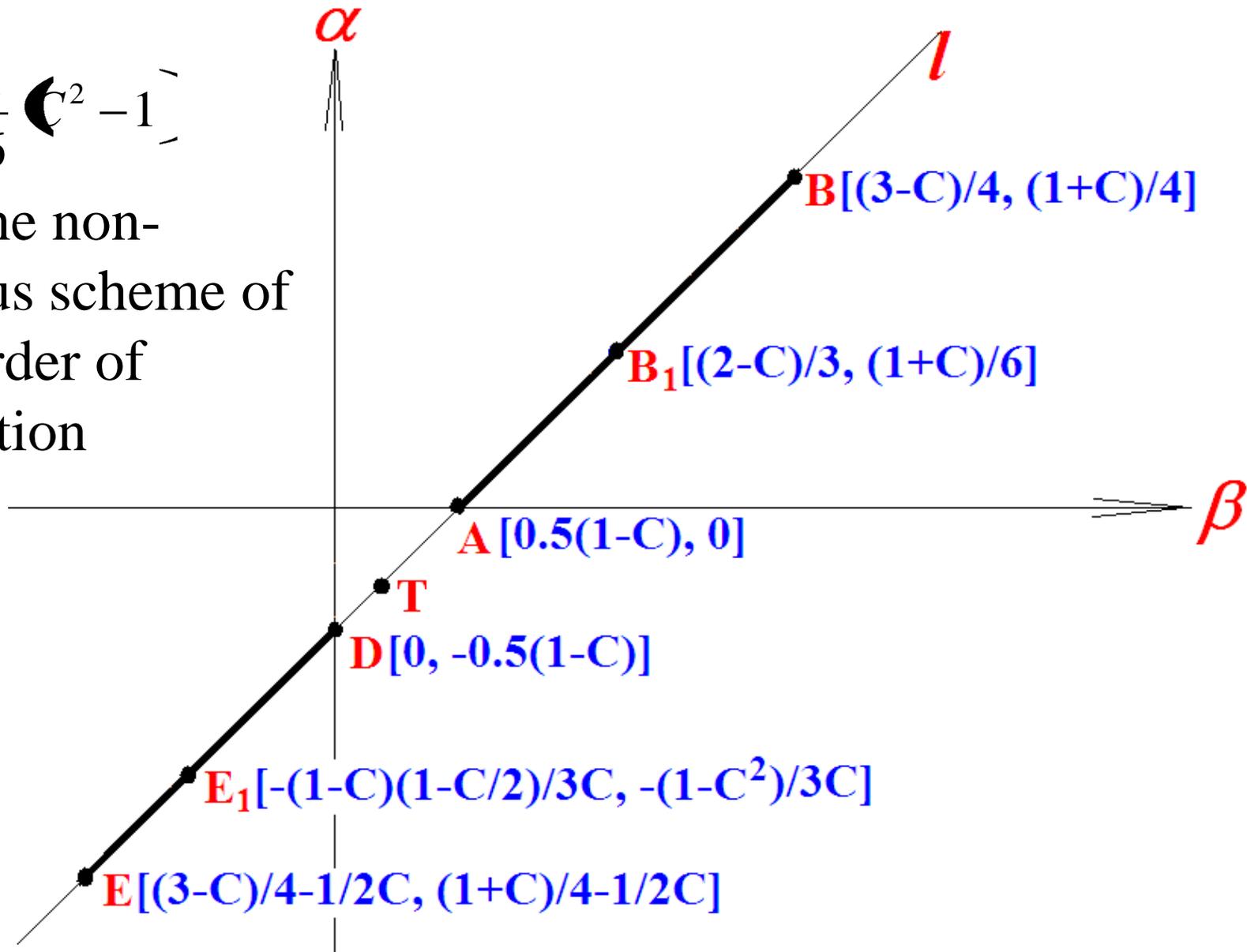
Therefore we can use the following switch condition between MCDS and MUDS: $(u \cdot \Delta f \cdot \Delta^2 f).$

At $(u \cdot \Delta f \cdot \Delta^2 f) \leq 0$ we use MCDS from AB_1 ,

At $(u \cdot \Delta f \cdot \Delta^2 f) > 0$ – MUDES from E_1D .

At $\alpha = \frac{1}{6}(C^2 - 1)$

we have one non-monotonous scheme of the third order of approximation (point **T**).



The first order - 1- $O(\tau, h)$ (Godunov S.K.):

$$\alpha = 0, \beta = 0,$$

$$f_i^{n+1} = f_i - C (f_i - f_{i-1}).$$

The second order - 2- $O(\tau^2, h^2)$ - Mac-Cormak:

$$\alpha = 0, \beta = 0.5 (1 - C),$$

$$f_i^{n+1} = f_i - 0.5 \cdot C (f_{i+1} - f_{i-1}) + 0.5 \cdot C^2 (f_{i+1} - 2f_i + f_{i-1}).$$

The third order - 3- $O(\tau^2, h^3)$ - Kholodov A.S.-
nonmonotonous:

$$\alpha = -0.25 (1 - C), \beta = 0.25 (1 - C),$$

$$f_i^{n+1} = f_i - C (f_i - f_{i-1}) + 0.25 \cdot C (1 - C) (f_{i+1} - f_i - f_{i-1} + f_{i-2}).$$

The scheme of the third order of accuracy - 4- $O(\tau^3, h^3)$:

$$\alpha = (C^2 - 1)/6, \beta = (1 - C) (2 - C)/6,$$

$$f_i^{n+1} = f_i - C (f_i - f_{i-1}) + C^2 (f_{i+1} - f_{i-1}) - C^3 (f_{i+1} - 2f_i + f_{i-1}).$$

The scheme of the third order of accuracy $O(\tau^3, h^3)$:

$$\alpha = (C^2 - 1)/6, \beta = (1 - C)(2 - C)/6,$$

$$f_i^{n+1} = f_i - C(f_i - f_{i-1}) - \frac{C}{6}(2 - C)(-C)f_{i+1} + \frac{C}{2}(-C)^2 f_i + \frac{C^2}{2}(-C)f_{i-1} + \frac{C}{6}(C^2 - 1)f_{i-2}$$

The hybrid scheme of the second order $O(\tau^2, h^2)$ with zero scheme viscosity and monotonous:

at $(u \cdot \Delta f \cdot \Delta^2 f) \leq 0$ MCDS: $\alpha = 0, \beta = 0.5(1 - C)$,

$$f_i^{n+1} = -0.5 \cdot C(1 - C) f_{i+1} + (-C^2) f_i + 0.5 \cdot C(+C) f_{i-1}, \quad u \geq 0,$$

$$f_i^{n+1} = -0.5 \cdot C(1 + C) f_{i+1} + (+C^2) f_i + 0.5 \cdot C(-C) f_{i-1}, \quad u < 0,$$

and at $(u \cdot \Delta f \cdot \Delta^2 f) > 0$ MUDS: $\alpha = -0.5(1 - C), \beta = 0$,

$$f_i^{n+1} = (-0.5 \cdot C(3 - C)) f_i + C(-C) f_{i-1} - 0.5 \cdot C(-C) f_{i-2}, \quad u \geq 0,$$

$$f_i^{n+1} = (+0.5 \cdot C(3 - C)) f_i - C(-C) f_{i+1} + 0.5 \cdot C(-C) f_{i+2}, \quad u < 0.$$

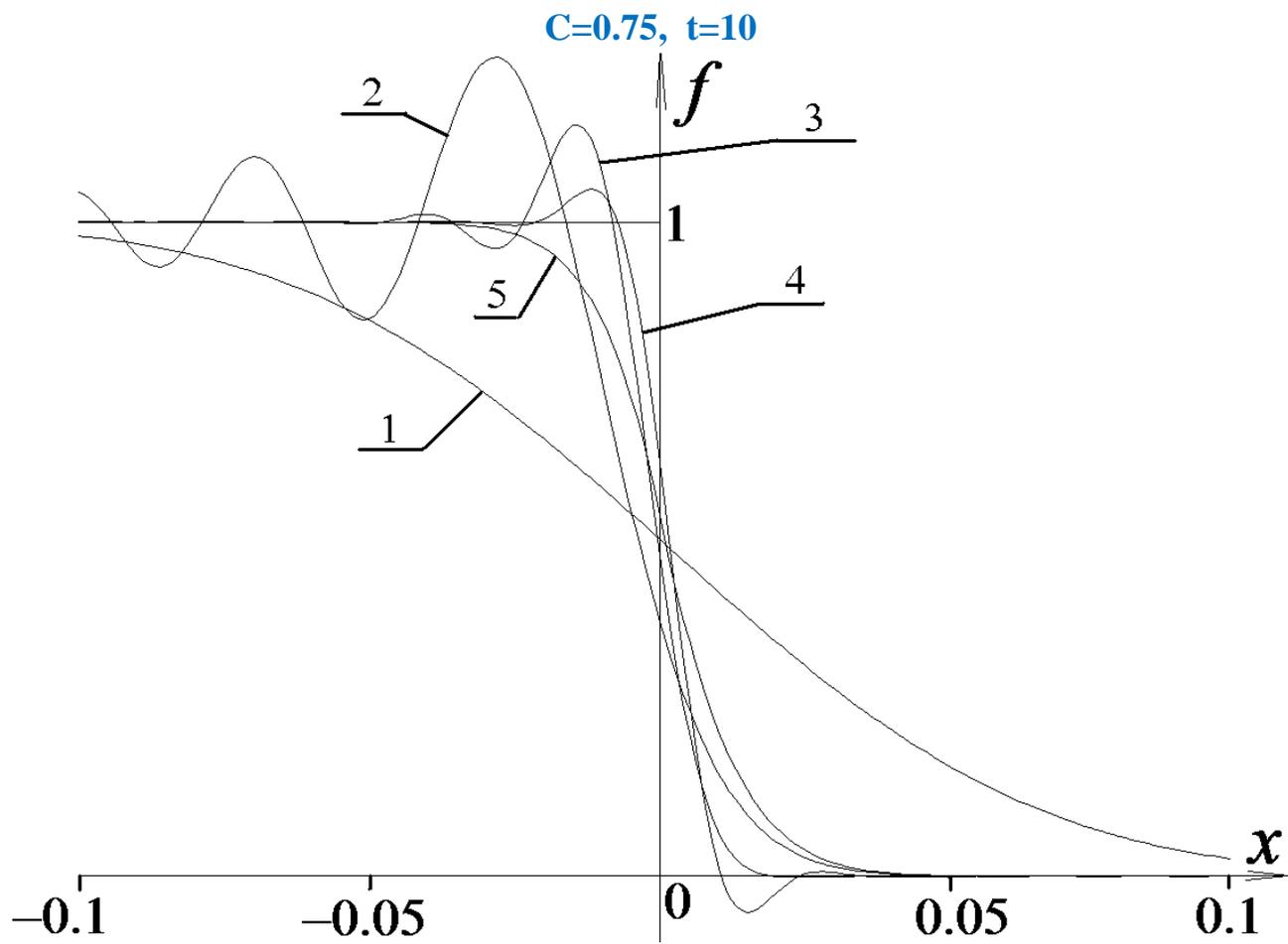
The solution of Cauchy problem

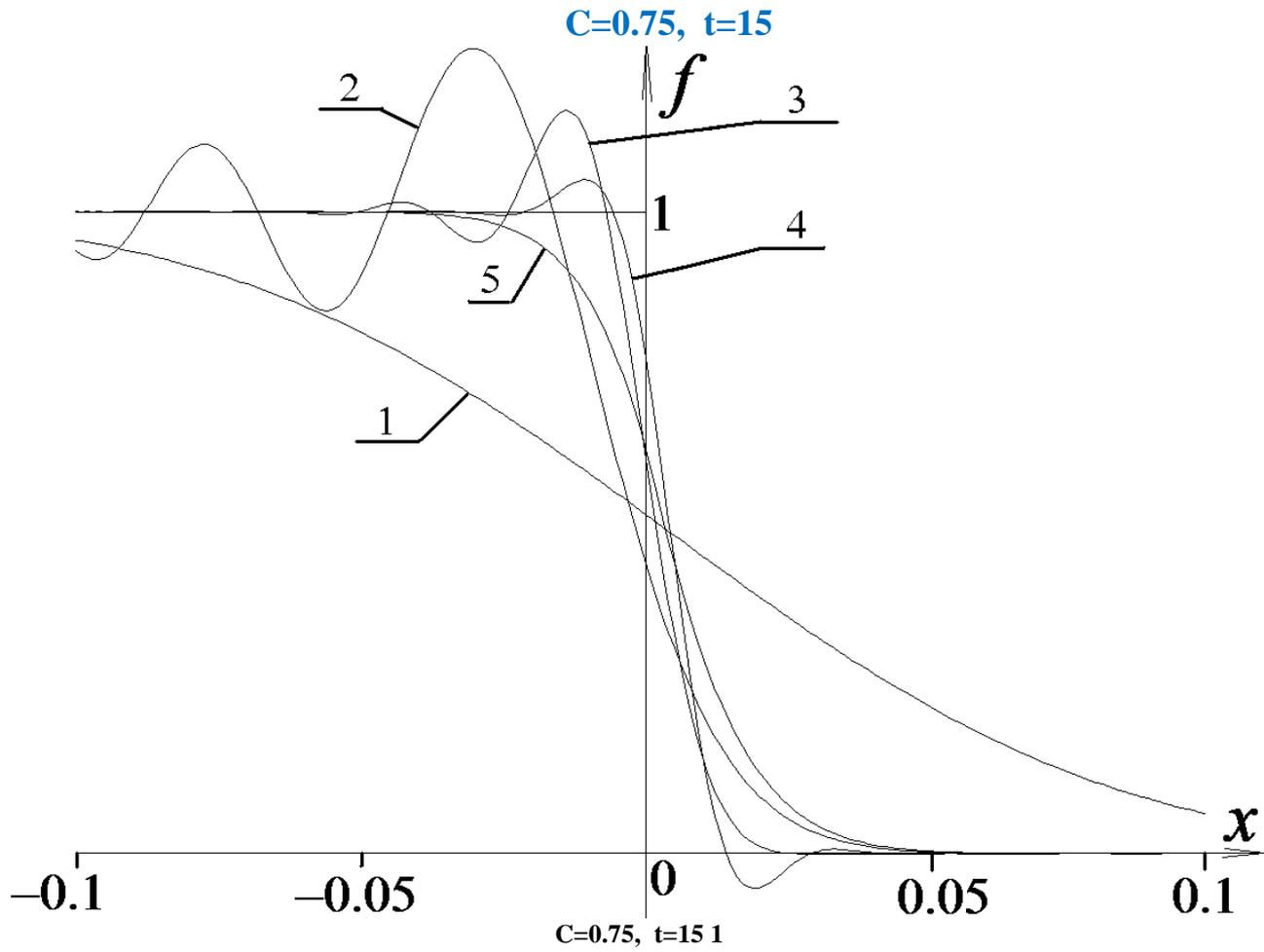
$$f_t + u f_x = 0, \quad u = \text{const} = 1,$$

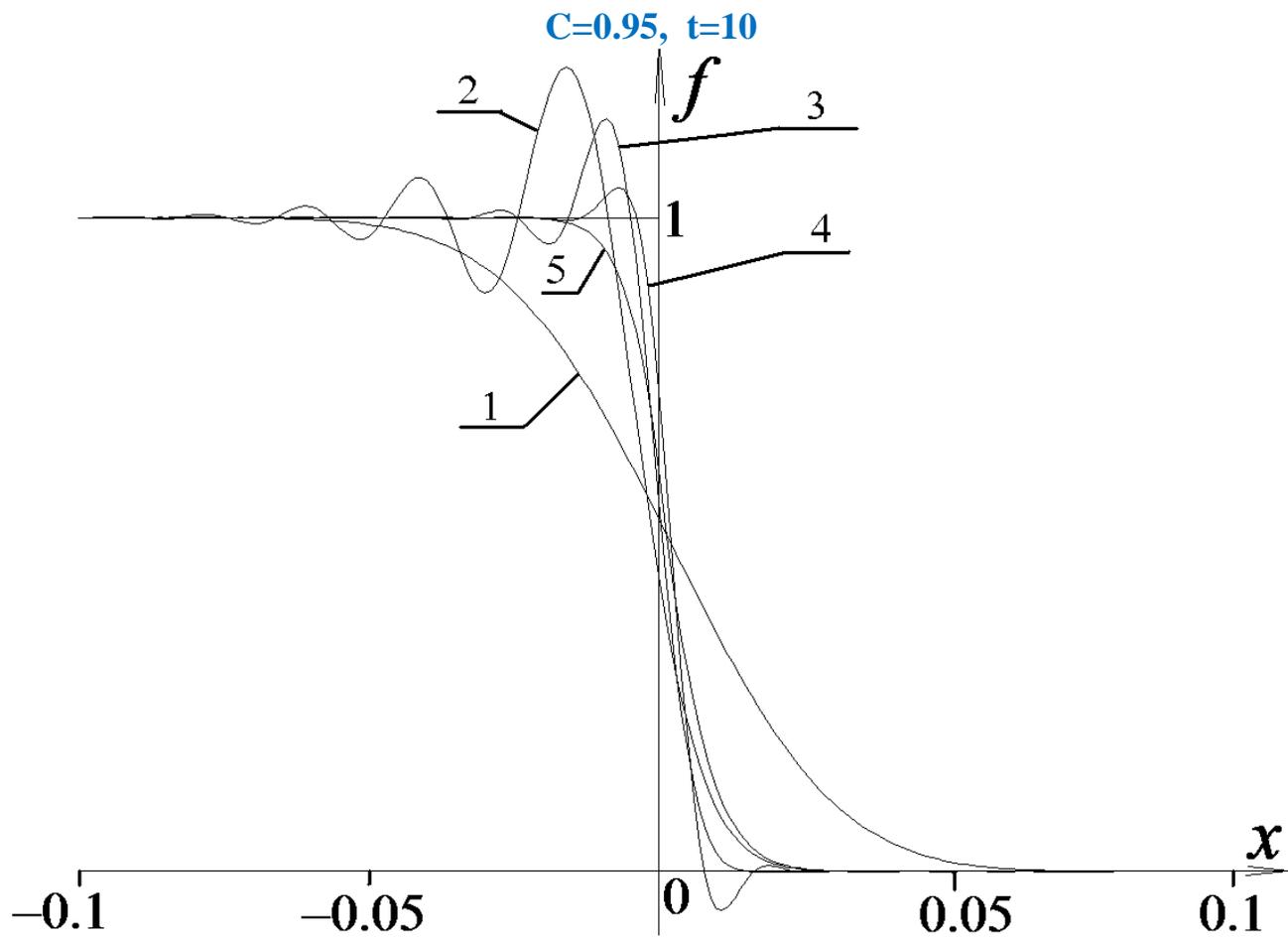
$$f(x, 0) = \begin{cases} 1, & x \leq 0 \\ 0, & x > 0 \end{cases}; \quad f(0, t) = 1, \quad f(\infty, t) = 0 \quad \text{при любом } t;$$

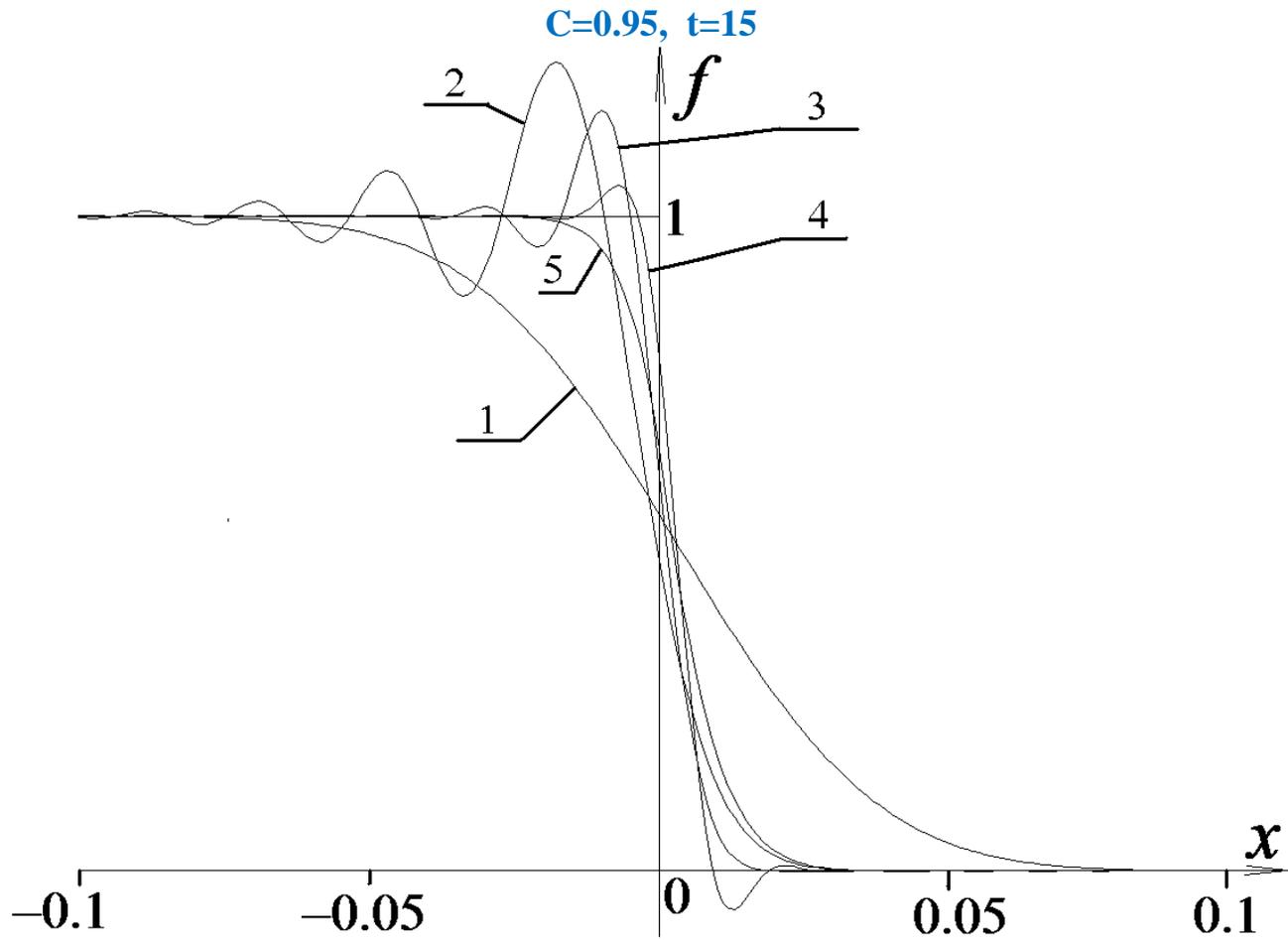
at $t = 10$ and $t = 15$,

$C = u \tau / h = 0.75$, $h = 0.001$ see in figs.



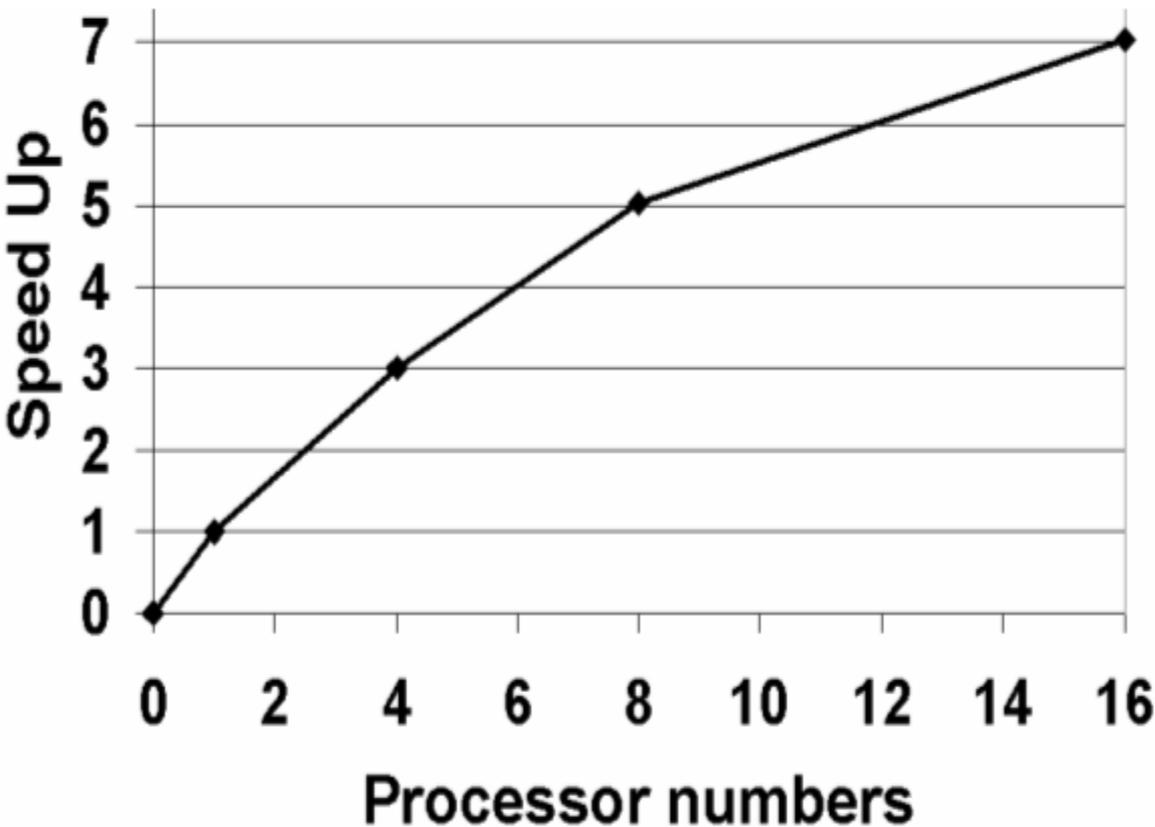






CODE PARALLELIZATION

The code has been parallelized by using **domain decomposition in the radial direction**. The computational domain has been divided into spherical subdomains corresponding to the parallel processor units.



Speed up for the switch Myrinet-2000 (MVS-1000 based on Intel Xeon (2.4 GHz) processors) for computational grid 80x50x100.

Let us consider a local stream line pattern around any point in a flow in a reference frame moving with the velocity of that point:

β — visualization

$$\dot{\vec{x}} = \mathbf{G} \vec{x} + O(|\vec{x}|^2)$$

The characteristic equation for the eigen-values σ of the velocity gradient tensor $\mathbf{G} = V_{i,j}$:

$$\sigma^3 - P \sigma^2 + Q \sigma - T = 0$$

The discriminant of this equation: $\Delta = (Q/3)^3 + (T/2)^2$

The condition $\Delta > 0$ at some point in a flow means that

two eigen-values $\sigma_{1,2} = \alpha \pm i \beta$ of \mathbf{G} are complex and the local streamline pattern is closed (at $\alpha = 0$) or spiral in a reference frame moving with this point. $\beta = \text{Im}(\sigma_{1,2})$ is the angular velocity of this spiral motion.

A vortex core is a connected regions with $\beta > 0$

Navier – Stokes equ. gradient: $a_{i,j} = -p_{,ij} + \frac{u_{i,jkk}}{Re}$ (1)

$$u_{i,j} = \frac{\partial u_i}{\partial x_j} = \frac{1}{2}(u_{i,j} + u_{j,i}) + \frac{1}{2}(u_{i,j} - u_{j,i}) = S_{ij} + \Omega_{ij}$$

Jeong J., Hussain F. On the identification of a vortex. J. Fluid Mech., 1995, V. 285.

$$\frac{DS_{ij}}{Dt} + S^2 + \Omega^2 = -\frac{\partial^2 p}{\partial x_i \partial x_j} + \frac{S_{ij,kk}}{Re}$$

λ_2 –visualization:

A vortex core is a connected region with two negative eigenvalues of $S^2 + \Omega^2$

$$(\lambda_2 < 0) \quad (\lambda_1 \geq \lambda_2 \geq \lambda_3).$$

(i) Unsteady straining can create a pressure minimum without involving a vortical or swirling motion.

(ii) Viscous effects can eliminate the pressure minimum in a flow with vortical motion.

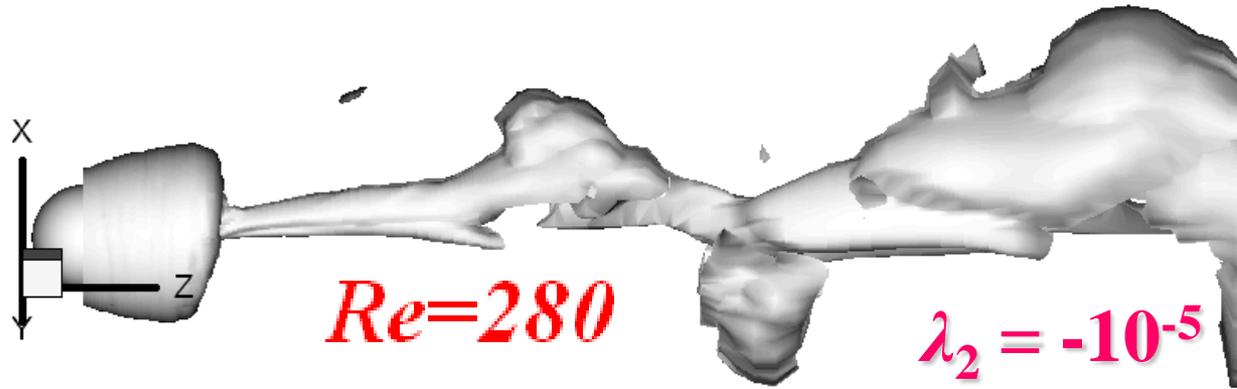
Режимы течения:

I) $20.5 < Re \leq 200$ –

однонитевой след

II) $200 < Re \leq 270$ –

двухнитевой след



III) $270 < Re \leq 400$ – периодический отрыв верхнего края
вихревой оболочки

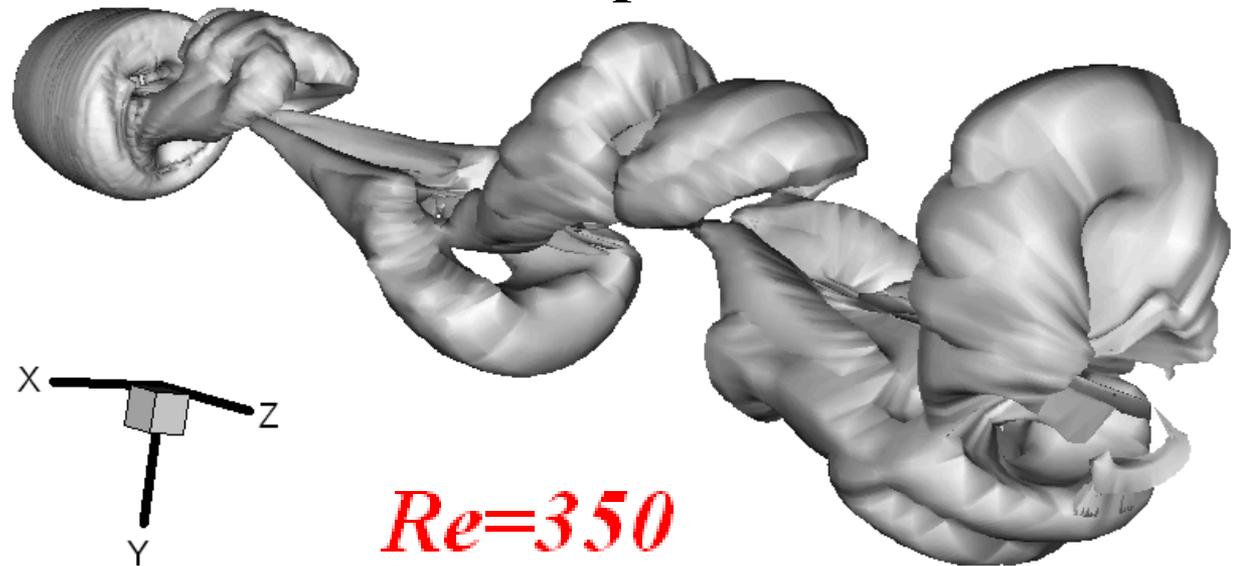
a) $270 < Re \leq 290$

b) $290 < Re \leq 320$

c) $320 < Re \leq 400$

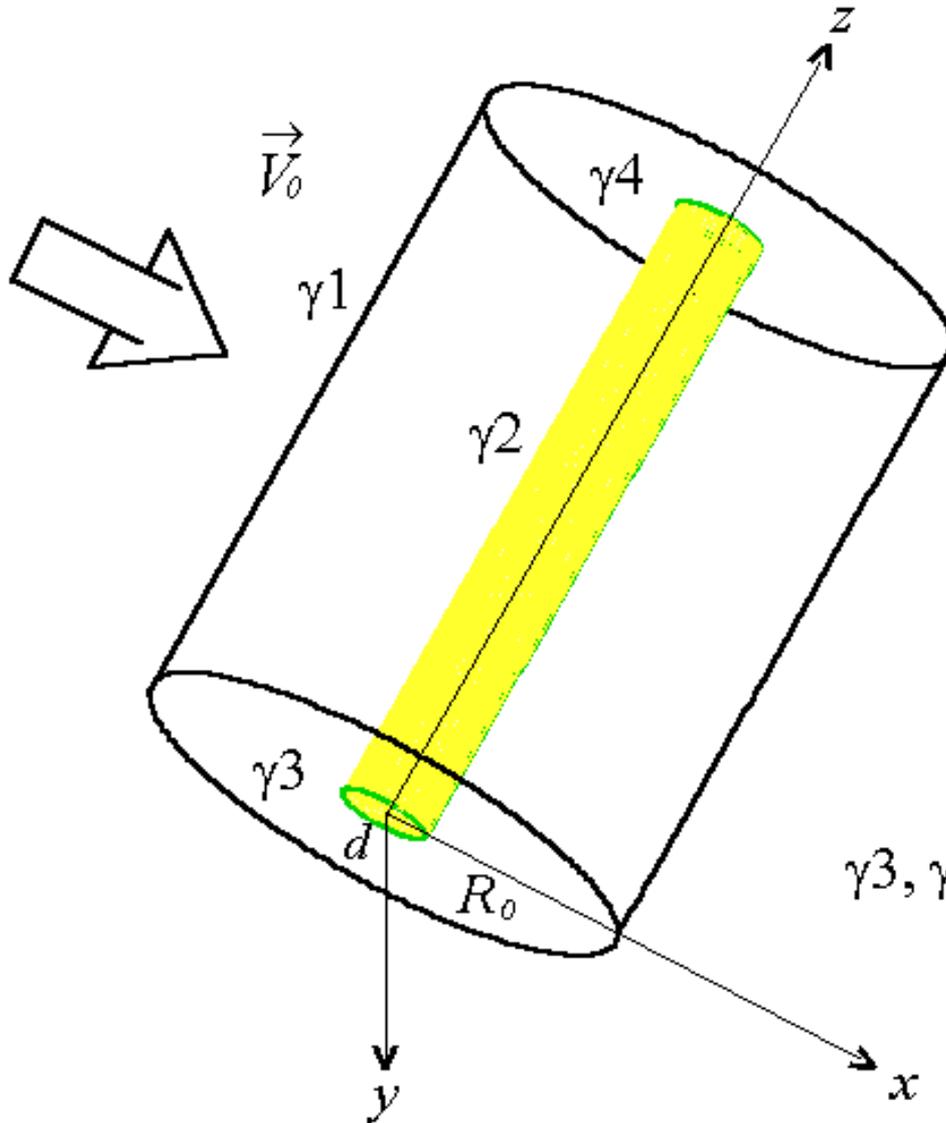
d) $360 < Re \leq 400$ –

регулярное вращение вихревой оболочки



3D Circular Cylinder.

Foundation of the problem

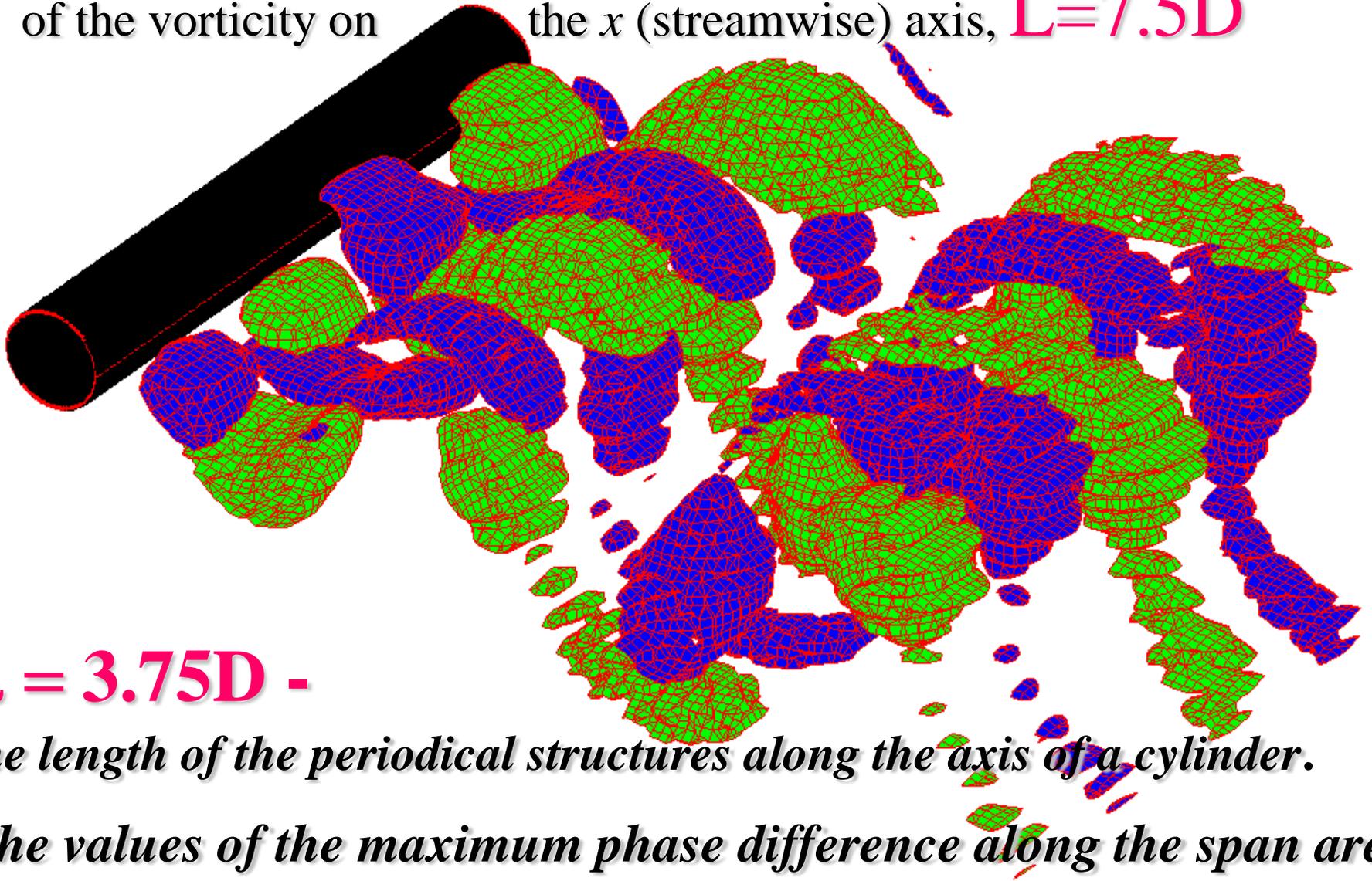


Boundary conditions:

γ_3, γ_4 : *periodical conditions*

Re=230, Mode A, Isosurfaces of the projection

of the vorticity on the x (streamwise) axis, $L=7.5D$

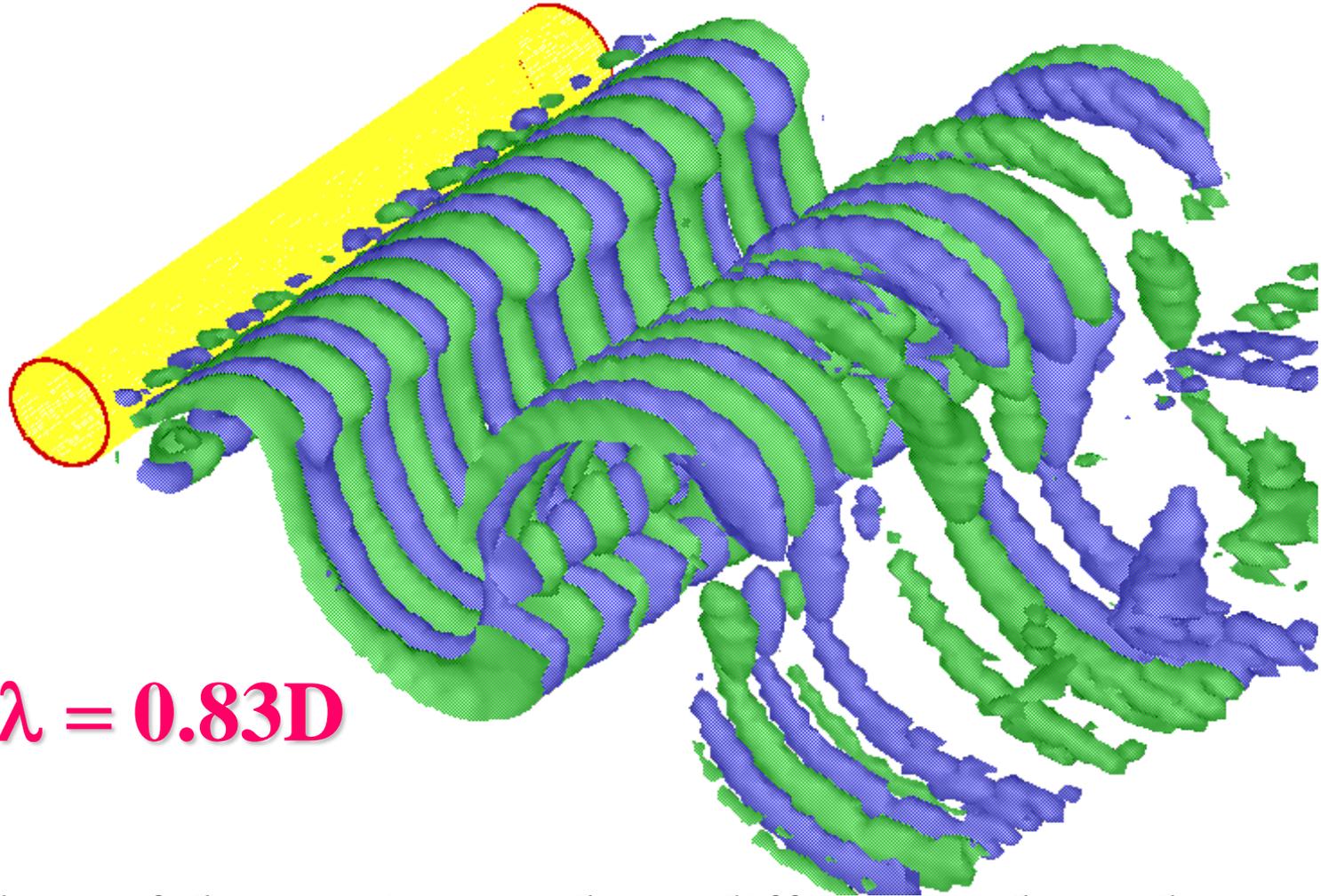


$\lambda = 3.75D$ -

the length of the periodical structures along the axis of a cylinder.

The values of the maximum phase difference along the span are approximately equal to $0.1-0.2 T$, where T is the flow period.

Re=320, Mode B, *Isosurfaces of the projection of the vorticity on the x (streamwise) axis, L=7.5D*



$$\lambda = 0.83D$$

The values of the maximum phase difference along the span are approximately equal to 0.015-0.030 T, where T is the flow period.

Literature

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Conclusions

1. The hybrid (second order of accuracy, possesses by zero scheme viscosity and monotonic) scheme has been constructed on the basis of MCDS and MUDS for approximation of the convective terms of the full CFD-equation.
2. The efficiency of this scheme have been demonstrated on the example of simulation of **2D-3D transitional flow regimes in the wake of a sphere and a circular cylinder.**

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