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Декомпозиция процесса решения задач аэродинамики по времени и по заданиям

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The digital wind tunnel is the worthy problem for scientific computing

- “Computational fluid dynamics has become a key technology in the development of new products in the aeronautical industry.” But up to now computational algorithms do not produce sufficiently accurate results which are needed for industry despite the great performance of computers.

The digital wind tunnel

The direct solving this Problem requires computers of huge performance. For example, to analyze sound effects. Sound speed equals 330 m/s, the upper bound of frequency is 20 kHz with wave length 1.65 cm. To analyze sound propagation, one have to take the characteristic size of a grid (for approximation) at least 1/6 of wave length, i.e., 0.275 cm and time step $8 \cdot 10^{-6}$ s. One cubic meter contains $1.75 \cdot 10^{8}$ cubes with such edge. But we need analyze tens 10^{3} cubic meter at least during 1 second of flying. Every cell takes 10^{3}-10^{4} arithmetical operations for one time step but number of these steps is greater $1.25 \cdot 10^{5}$. Therefore it needs 10^{22} arithmetical operations. The performance of modern computers is 10^{15} Flop/s. It means 10^{7} s, i.e., 116 days with the best computer and coding for poor accuracy.

The digital wind tunnel

- The goal of Project “Tristam” is to develop and utilize innovative adaptive high-order computational methods for compressible flow equations for large-scale aerodynamic applications in aircraft design.

Contents of talk

- 1. Three stages of solving process for the problem
  - 1.1. Navier-Stokes equations in two-dimensional case as illustration
  - 1.2. First stage: "Input and Preliminary Solving"
  - 1.3. Second stage: "The Prepack"
  - 1.4. Third stage: “The Goal-Oriented Task”
- 2. New and adapted numerical approaches
  - 2.1. Solution of continuity equation. Approximation along trajectories
  - 2.2. Defect correction method in general sense
  - 2.3. Substitution of unknown function in energy equation
  - 2.4. Accuracy and superconvergence
  - 2.5. Usage of computer architecture: CPU + GPU

Project “Tristam”

- We suggest to develop the process of solving three-dimensional aerodynamic problems, which consists of three stages, may be performed and repeated in different places at corresponding computer systems and architectures with different required tasks and appropriate accuracy.

Input and Preliminary Solving

- The first stage "Input and Preliminary Solving" consists of formulation of geometry, storing data, and solving the Problem on the almost uniform grid coordinated with the surface of a body.

  Nevertheless even at this initial stage we suggest new numerical methods of fourth order of accuracy, which combine finite element method in space, finite difference method in time, and defect correction method to improve accuracy.

"The Prepack"

- The second stage "The Prepack" consists of three steps. First step analyzes the solution of first stage and finds out vicinities of possible problematic areas with greater gradients (shock and boundary layers, etc).

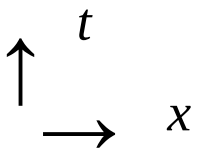
Temporal estimator

- Estimator of order k:

$$E = D_l^k f = \frac{\partial^k f}{\partial l^k}(\xi)$$

where difference derivative of order k along some trajectory equals partial derivative of the same order in the direction of this trajectory

$$f := \rho,\ \sigma u,\ \sigma v,\ \rho\eta$$



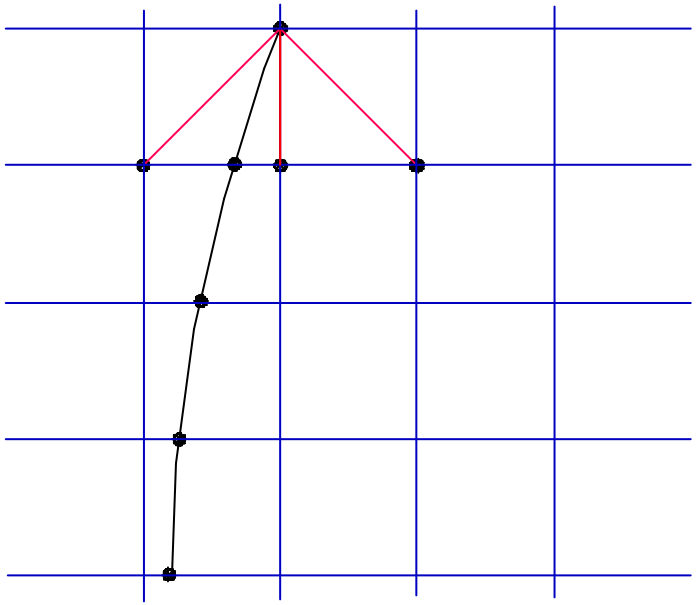


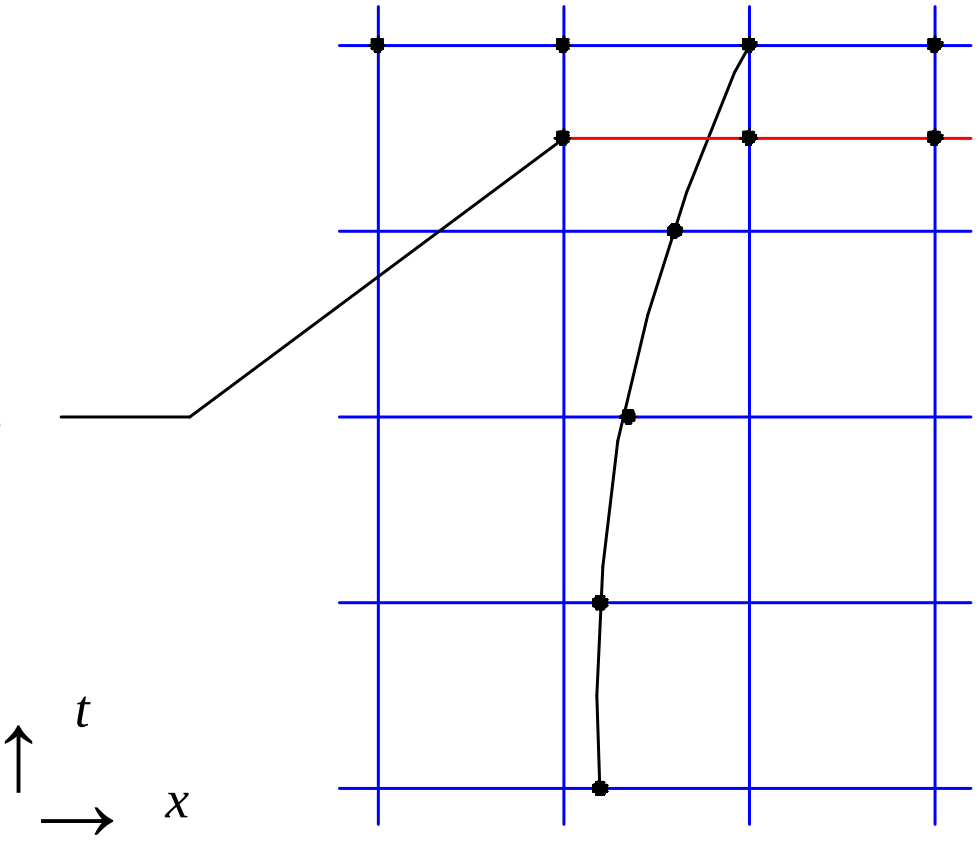
Fig. 2. Black line demonstrates trajectory with nodes of high-order differences.

Temporal adaptivity

Adaptivity:

The greater $|E|$ the less Δt.

interpolated node



That is

$$\Delta t_{local} = e_{opt} \Big/ \left| E_{local} \right|$$

with given temporal parameter e_{opt} .

Fig. 2. Black line demonstrates trajectory with initial nodes for estimator.

Spatial mean-value estimator

- Estimator of fourth order begins with matrix

$$\begin{pmatrix} D_x^4 & D_x^2 D_y^2 & D_x^2 D_z^2 \\ D_x^2 D_y^2 & D_y^4 & D_y^2 D_z^2 \\ D_x^2 D_z^2 & D_y^2 D_z^2 & D_z^4 \end{pmatrix} f = \begin{pmatrix} \frac{\partial^4 f}{\partial x^4} & \frac{\partial^4 f}{\partial x^2 \partial y^2} & \frac{\partial^4 f}{\partial x^2 \partial z^2} \\ \frac{\partial^4 f}{\partial x^2 \partial y^2} & \frac{\partial^4 f}{\partial y^4} & \frac{\partial^4 f}{\partial y^2 \partial z^2} \\ \frac{\partial^4 f}{\partial x^2 \partial z^2} & \frac{\partial^4 f}{\partial y^2 \partial z^2} & \frac{\partial^4 f}{\partial z^4} \end{pmatrix}$$

where D_x^4 is the fourth difference derivative, for example,

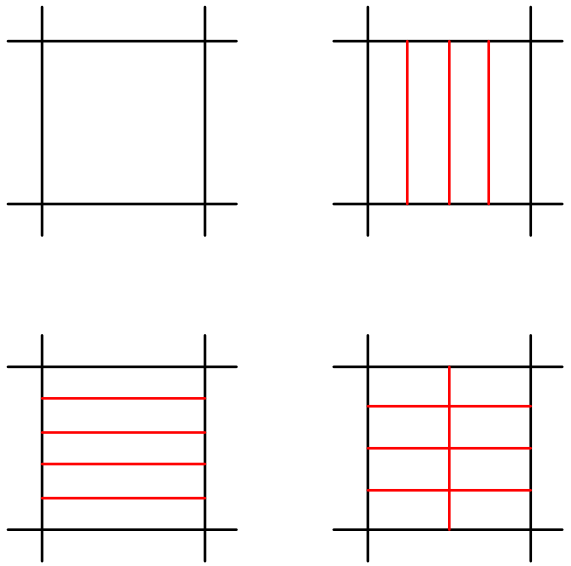
$$D_x^4 f(x) = (f(x-2h) - 4f(x-h) + 6f(x) - 4f(x+h) + f(x+2h))/h^4$$

Spatial mean-value estimator

- Then we compute 3 real eigenvalues $\lambda_1, \lambda_2, \lambda_3,$ and 3 eigenvectors ν_1, ν_2, ν_3 of this matrix

- Comparison of absolute values with given spatial parameter d_{opt}^4 gives the multiplier of mesh condensation $d_{opt}^4 / |\lambda_i|$ in each direction ν_1, ν_2, ν_3

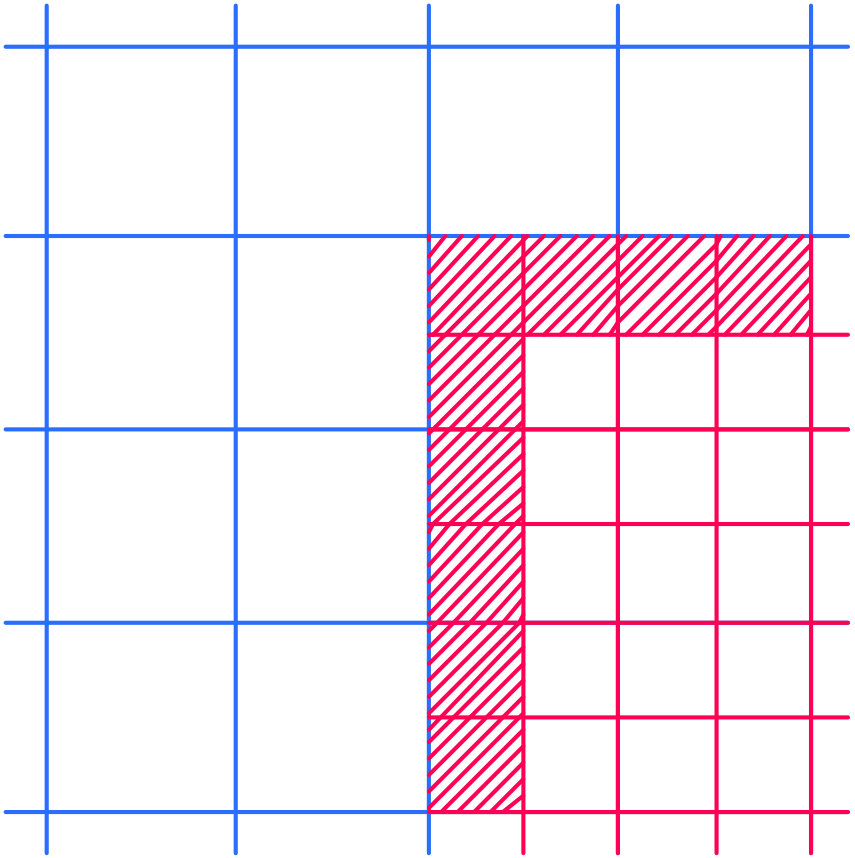
- So we can get different situation subject to directions:



"The Prepack"

- Second step modifies the triangulation: makes it condensed in the vicinity of problematic areas and more sparse in the areas of smooth behavior of the previous solution. The computational domain may be slightly reduced.

Conforming finite elements



After condensation of meshes the transparent red elements have the same set of degrees of freedom as blue ones (only with other scale) except hatched meshes with incomplete set of degrees of freedom.

"The Prepack"

- At the third step the Problem is solved again on the modified triangulation and this solution is stored and used later as the “prepack” for many other tasks and other computers. For some Problems several iterations of the second stage may be repeated for better accuracy.

The Goal-Oriented Task-1: computing important parameters

- The third stage “The Goal-Oriented Task” also consists of three steps. Special task may means the calculation of one of the important parameters: drag, lift, moment coefficient, etc. At first, on the previous constructed (second) triangulation another Problem is solved which is adjoint to the previous linearized equations in the sense of corresponding cost functional.

The Goal-Oriented Task-1: computing important parameters

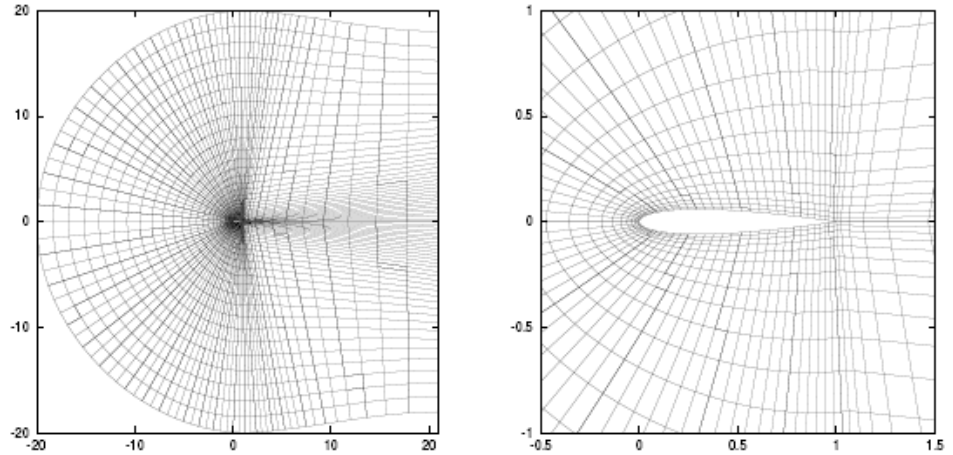
- The solution of adjoint problem (as function of sensitivity for our functional) gives information for further reconstruction of triangulation.

The Goal-Oriented Task-1: computing important parameters

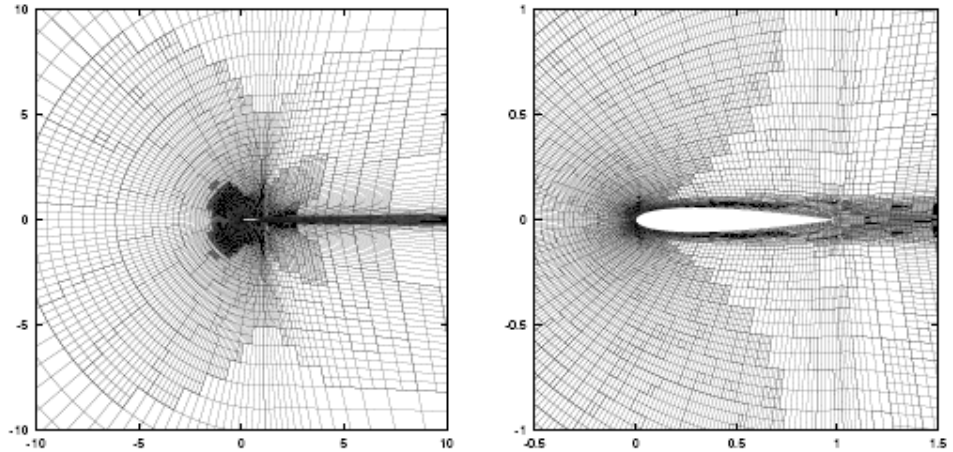
- At the third step the initial required Problem is solved at new (already the third) triangulation.

The Goal-Oriented Task-1: computing important parameters

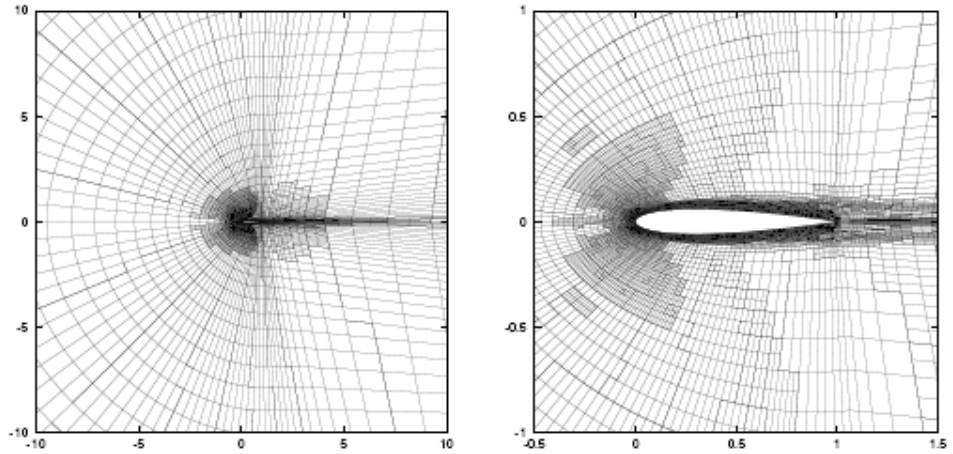
- As a example look at this approach in stationary two-dimensional Navier-Stokes problem from paper by R. Hartmann in the framework of Project ADIGMA.



Initial triangulation
~ 3000 elements
~ 43000 degrees of freedom
accuracy 0.02
for pressure drag



Second triangulation
~ 30000 elements
~ 560000 degrees of freedom
after second stage
accuracy 0.0016



Third triangulation
~ 35000 elements
~ 560000 degrees of freedom
after third stage
accuracy $2 \cdot 10^{-5}$

The Goal-Oriented Task-2: implementation to other physical process

- After second stage one gets numerical solution of problem (pressure, velocity) with appropriate accuracy for other physical process. If these processes influence the solution, one can repeat the computations with new data at second triangulation.

The Goal-Oriented Task-2: implementation to other physical process

- For example, the finite element solution gives not bad averaged flow for acoustics. After second stage one can repeat computations by defect correction method in some sufficiently small regions where sound is generated.

The Goal-Oriented Task-3: solution of inverse problems

- Any mathematical model contains many numerical parameters (or even functions) which are known approximately. Sometimes their accuracy is not sufficient and produces an additional error that lowers model quality. Of course, these parameters may be improved by real experiments or by extrapolation of physical laws. In any case it takes some physical experiments.
- But we can try to solve problem with known excess indirect data and to improve this parameters by mathematical way. In this case we take cost functional as the norm of difference between real and current values of these indirect data.

Navier-Stokes equations

Let $\Omega = (0,1) \times (0,1)$ be a bounded (computational) domain in R^2 with the boundary Γ.

Let also $(0, t_{fin})$ be the time interval. Consider the problem on a nonstationary flow of a viscous heat-conducting gas in the following form.

2D Navier-Stokes equations

In the cylinder $(0, t_{fin}) \times \Omega$ we write four equations in unknowns $\rho,\ u,\ v,\ e$:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0, \tag{1}$$

$$\left(\rho\frac{\partial u}{\partial t} + \frac{u}{2}\frac{\partial \rho}{\partial t}\right) + \left(\rho u\frac{\partial u}{\partial x} + \frac{u}{2}\frac{\partial}{\partial x}(\rho u)\right) + \left(\rho v\frac{\partial u}{\partial y} + \frac{u}{2}\frac{\partial}{\partial y}(\rho v)\right)$$

$$+\frac{\partial P}{\partial x} - \frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{xy}}{\partial y} = 0, \tag{2}$$

$$\left(\rho\frac{\partial v}{\partial t} + \frac{v}{2}\frac{\partial \rho}{\partial t}\right) + \left(\rho u\frac{\partial v}{\partial x} + \frac{v}{2}\frac{\partial}{\partial x}(\rho u)\right) + \left(\rho v\frac{\partial v}{\partial y} + \frac{v}{2}\frac{\partial}{\partial y}(\rho v)\right)$$

$$+\frac{\partial P}{\partial y} - \frac{\partial \tau_{xy}}{\partial x} - \frac{\partial \tau_{yy}}{\partial y} = 0, \tag{3}$$

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x}(e\rho u) + \frac{\partial}{\partial y}(e\rho v) + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = -P\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + \Phi. \tag{4}$$

Notation

$\rho(t,x,y)$ is density;

$u(t,x,y)$, $v(t,x,y)$ are components of the vector $\mathbf{u}$ of velocity;

$e(t,x,y)$ is internal energy of mass unit;

$P(t,x,y)$ is pressure;

$\tau_{xx}, \tau_{xy}, \tau_{yy}$ are the components of the stress tensor $\mathcal{T}$:

$$\tau_{xx} = \frac{2}{3}\mu\left(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right),\ \tau_{yy} = \frac{2}{3}\mu\left(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x}\right),\ \tau_{xy} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right);$$

$$\mu(t,x,y) = \frac{1}{Re}\mu^*(t,x,y),$$

μ^* is the dynamic coefficient of viscosity:

$$\mu^* = \left((\gamma-1)\gamma \mathrm{M}_\infty^2\right)^\omega e^\omega, \quad 0.76 \le \omega \le 0.9; \tag{5}$$

(q_x, q_y) are components of the vector $\mathbf{q}$ of density of a heat flow given by the formulae:

$$q_x(t,x,y) = -\frac{\gamma}{\mathsf{Pr}}\mu\frac{\partial e}{\partial x}, \quad q_y(t,x,y) = -\frac{\gamma}{\mathsf{Pr}}\mu\frac{\partial e}{\partial y};$$

Re is the Reynolds number; Pr is the Prandtl number;

M_∞ is the Mach number; γ is a gas constant.

The equation of state has the form:

$$P = (\gamma - 1)\rho e.$$

The dissipative function Φ will be considered in the following form:

$$\Phi = \mu\left(\frac{2}{3}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{2}{3}\left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)^2 + \frac{2}{3}\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)^2\right). \quad (6)$$

From (6) it follows that it is nonnegative.

The solution of continuity equation. Why differentiation along trajectories?

- Solution of this equation is smooth only along its characteristics and is not liable to be smooth in any different direction. Of course, in real situations there are no discontinuities but instead the great gradients and great derivatives appear in some directions.

- Therefore we shall treat approximation along characteristics with application of defect corrections to increase order of accuracy.

- The main idea consists in use of simple stable monotone scheme of first order of accuracy with consequent defect corrections by high-order differences along characteristics and by improvement of coefficients field.

Initial finite-difference scheme and high-order defect correction in 1D case

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0:$$

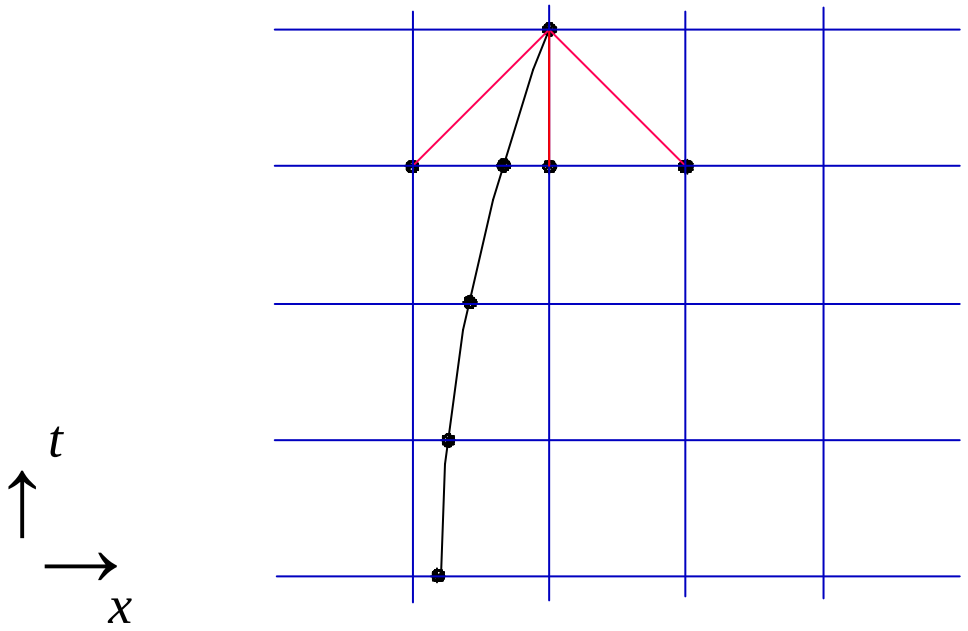


Fig. 1. Stencils for initial scheme and defect correction.
Red lines combine initial finite difference stencil.
Black line demonstrates characteristics with nodes of high-order differences.

Defect correction: general approach

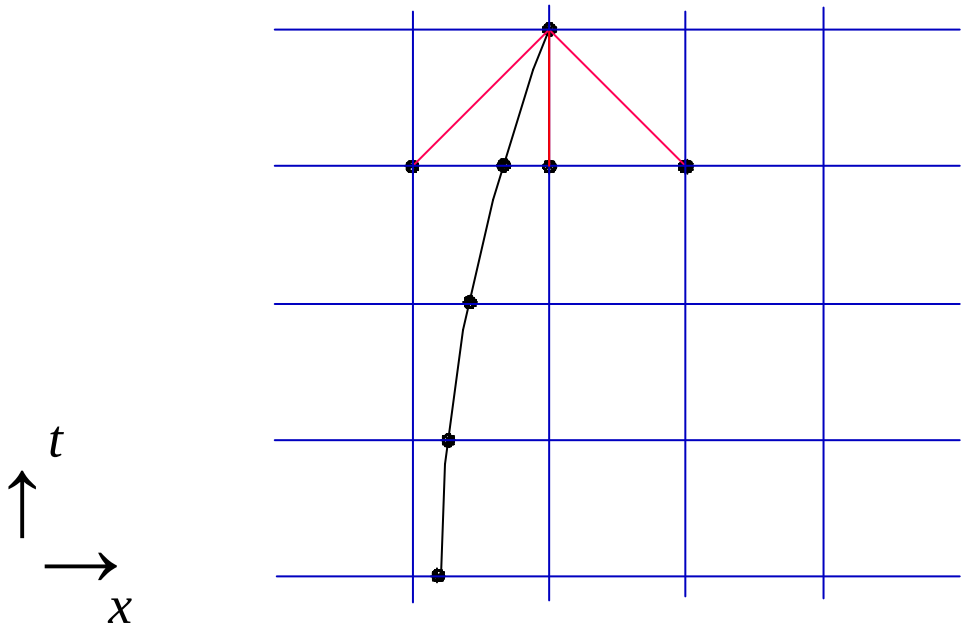
- $A^h u^h = f^h$ – stable finite-difference scheme of low order
- $L^h v^h = f^h$ – (unstable) finite-difference scheme of high order

Defect correction iterations:

- $u^0 = u^h$ where u^h is the solution to the stable scheme;
- $A^h u^{k+1} = f^h - L^h u^k + A^h u^k, \qquad k = 0, 1, 2.$

Initial finite-difference scheme and high-order defect correction in 1D case

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0:$$



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Red lines combine initial finite difference stencil.
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Approximation of momentum equations

- Finite difference scheme (with subsequent defect correction) is suggested for inertial terms in combination with finite element method for the rest terms.
- For this purpose the equations are slightly modified for convergence in discrete analogue of L_2 – norm.
- Of coarse, it is possible to implement finite volume method. The convenient norm for convergence of discrete solution by this method is discrete analogue of L_1 – norm. It is natural for the formulation of momentum conservation.
- But simultaneously we need to solve energy equation for the stability of which we have unique formulation of conservation law with weighted L_2 – norm for component of velocity and L_1 – norm for energy.

Two conservation laws

Variation of momentum for gas in volume Ω with boundary Γ

$$\frac{\partial}{\partial t}\int\limits_{\Omega}\rho\mathbf{u}\,d\Omega=\int\limits_{\Gamma}\left(\rho\mathbf{u}\cdot(\mathbf{u}\cdot\boldsymbol{n})+P\,\boldsymbol{n}-\tau_{ij}\cdot\boldsymbol{n}\right)\,d\Gamma$$

Variation of full energy of gas in volume Ω with boundary Γ

$$\frac{\partial}{\partial t}\int\limits_{\Omega}E\,d\Omega=-\int\limits_{\Gamma}\left(E\mathbf{u}+P\mathbf{u}-\tau_{ij}\mathbf{u}+\mathbf{q}\right)\cdot\boldsymbol{n}\,d\Gamma$$

Thus we have the balance relation which describes variation of total energy of mass of gas enclosed in the volume Ω in time unit:

$$\frac{d}{dt}\int_{\Omega}\rho\left(e+\frac{u^2+v^2}{2}\right)d\Omega = -\int_{\Gamma}\rho\left(e+\frac{u^2+v^2}{2}\right)\mathbf{u}\mathbf{n}\,ds \quad (8)$$
$$-\int_{\Gamma}(P\mathbf{u}-\mathcal{T}\mathbf{u}+\mathbf{q})\,\mathbf{n}\,ds.$$

Here $\mathbf{n}(x,y)=(n_x(x,y),n_y(x,y))$ denotes a vector of the unit outer normal to Γ at a point (x,y).

Approximation of momentum equations

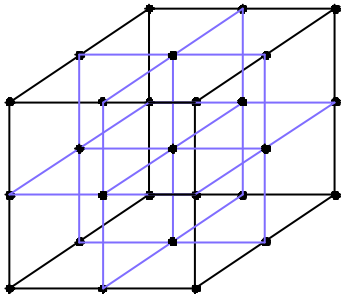
- Therefore it is more convenient to implement finite element method for component of velocity since discrete L_2 – norm is more natural for FEM.

- Since we can remove inertial terms out of variational formulation then we are able to implement traditional finite element method without any violations like upwind tricks and artificial viscosity.

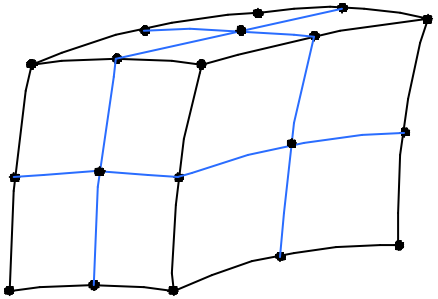
- Among different types of finite elements the triquadratic finite elements on hexahedrons including isoparametric ones are more attractive for our purposes.

Some properties for triquadratic finite elements

- First, curvilinear modification of triquadratic element exactly approximates curvilinear boundaries and transforms to standard cube.
- The quadrature nodes of Simpson-cubed formula are coincide with nodes of degrees of freedom, which results in lumping effect for right-hand side and absolute term. This formula gives forth order of accuracy in discrete L_2 – norm.



Rectangular triquadratic element



Curvilinear triquadratic element

Approximation properties of triquadratic finite elements

For considerably nonuniform meshes

$$\left\| u - u^I \right\|_0 \le ch^3 \left\| u \right\|_3$$
$$\left\| u - u^I \right\|_1 \le ch^2 \left\| u \right\|_3$$

It is expected that for quasi-uniform meshes with Jacobian matrix $J = I + h\,M$ between neighbouring elements

$$\left\| u^I - u^h \right\|_0 \le ch^4 \left\| u \right\|_4$$
$$\left\| u^I - u^h \right\|_1 \le ch^3 \left\| u \right\|_4$$

It is provided by Lin Q., Lin J. for biquadratic elements and some elliptic equations. Moreover for the interior of rectangular uniform mesh

$$\left\| u^I - u^h - h^4\varphi \right\|_0 \le ch^6 \left\| u \right\|_6$$
$$\left\| u^I - u^h - h^4\varphi \right\|_1 \le ch^5 \left\| u \right\|_6$$

where φ is some smooth function.

Domains of approximation are different for inertial terms and for other ones

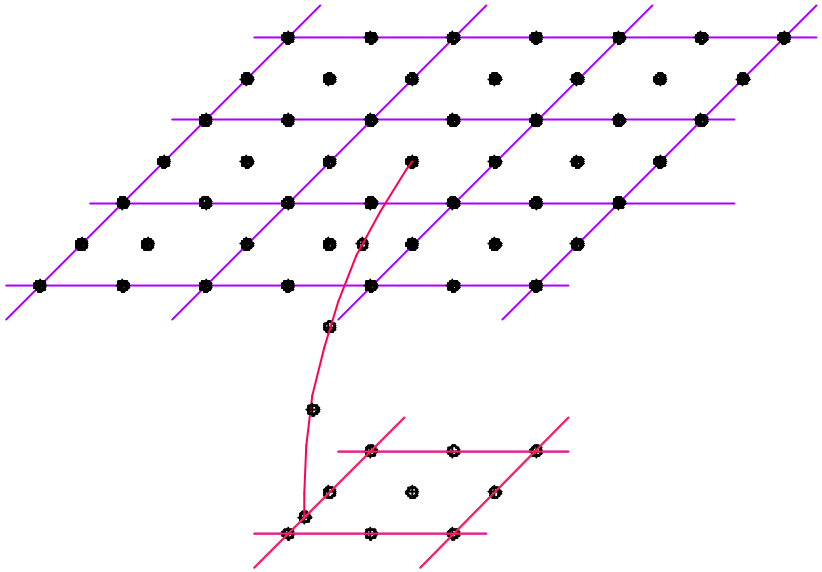


Fig. 2. Nodes on violet plane belong to unknown degrees of freedom in finite element method. Nodes on red curve and planes serve the known values for right-hand side in FEM.

Initial momentum equations

$$\rho\frac{\partial u}{\partial t}+\frac{u}{2}\frac{\partial \rho}{\partial t}+\frac{1}{2}\left(\frac{\partial}{\partial x}(\rho a u)+\rho a\frac{\partial u}{\partial x}\right)$$
$$+\frac{1}{2}\left(\frac{\partial}{\partial y}(\rho b u)+\rho b\frac{\partial u}{\partial y}\right)-\frac{\partial}{\partial x}(\tau_{xx})-\frac{\partial}{\partial y}(\tau_{xy})+\frac{\partial P}{\partial x}=0, \quad (18)$$

$$\rho\frac{\partial v}{\partial t}+\frac{v}{2}\frac{\partial \rho}{\partial t}+\frac{1}{2}\left(\frac{\partial}{\partial x}(\rho a v)+\rho a\frac{\partial v}{\partial x}\right)$$
$$+\frac{1}{2}\left(\frac{\partial}{\partial y}(\rho b v)+\rho b\frac{\partial v}{\partial y}\right)-\frac{\partial}{\partial x}(\tau_{xy})-\frac{\partial}{\partial y}(\tau_{yy})+\frac{\partial P}{\partial y}=0. \quad (19)$$

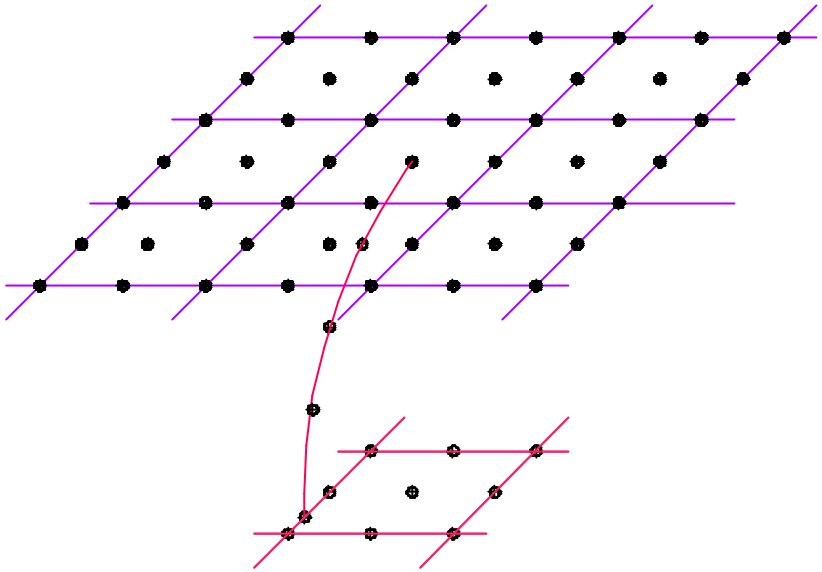
Reduced momentum equations at time level t

Due to approximation of inertial terms along characteristics, momentum equations at the time level t became simpler for finite element implementation (where Δt means temporal size):

$$\frac{\sigma u}{\Delta t} - \frac{\partial}{\partial x}(\tau_{xx}) - \frac{\partial}{\partial y}(\tau_{xy}) + \frac{\partial P}{\partial x} = f_u \tag{18}$$

$$\frac{\sigma v}{\Delta t} - \frac{\partial}{\partial x}(\tau_{xy}) - \frac{\partial}{\partial y}(\tau_{yy}) + \frac{\partial P}{\partial y} = f_v \tag{19}$$

Since domains of approximation are different for inertial terms and other ones it is possible to solve the problem on moving meshes



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Initial energy equation

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x}(e\rho u) + \frac{\partial}{\partial y}(e\rho v) + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = -P\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + \Phi. \tag{4}$$

Due to (9) and (10) we have

$$\int_\Omega \rho \left(e + \frac{u^2 + v^2}{2} \right) d\Omega = const. \tag{14}$$

Because of $\rho > 0$ we have some kind of conservation law where energy e enters in weighted L_1-norm and velocities do in L_2-norm. It produces great difficulties for stability of discretization. To simplify them let us introduce

$$e = \eta^2, \quad \text{i.e.,} \quad \eta = +\sqrt{e}. \tag{15}$$

And instead of (8) we get

$$\int_\Omega \rho \left(\eta^2 + \frac{u^2 + v^2}{2} \right) d\Omega = const, \tag{16}$$

that means the stability in weighted $L_2 \times L_2 \times L_2$-norm.

The conservation laws are sufficient for stability of differential problem and later in discrete form do for the difference scheme.

Transformed energy equation

$\eta = e^{1/2}$:

$$2\rho\frac{\partial\eta}{\partial t} + \eta\frac{\partial\rho}{\partial t} + \left(\frac{\partial}{\partial x}(\rho a\eta) + \rho a\frac{\partial\eta}{\partial x}\right) + \left(\frac{\partial}{\partial y}(\rho b\eta) + \rho b\frac{\partial\eta}{\partial y}\right)$$

$$- \frac{1}{\eta}\frac{\partial}{\partial x}\left(2\tilde{\mu}\eta\frac{\partial\eta}{\partial x}\right) - \frac{1}{\eta}\frac{\partial}{\partial y}\left(2\tilde{\mu}\eta\frac{\partial\eta}{\partial y}\right) + \frac{P}{\eta}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) - \frac{\Phi}{\eta} = 0. \quad (21)$$

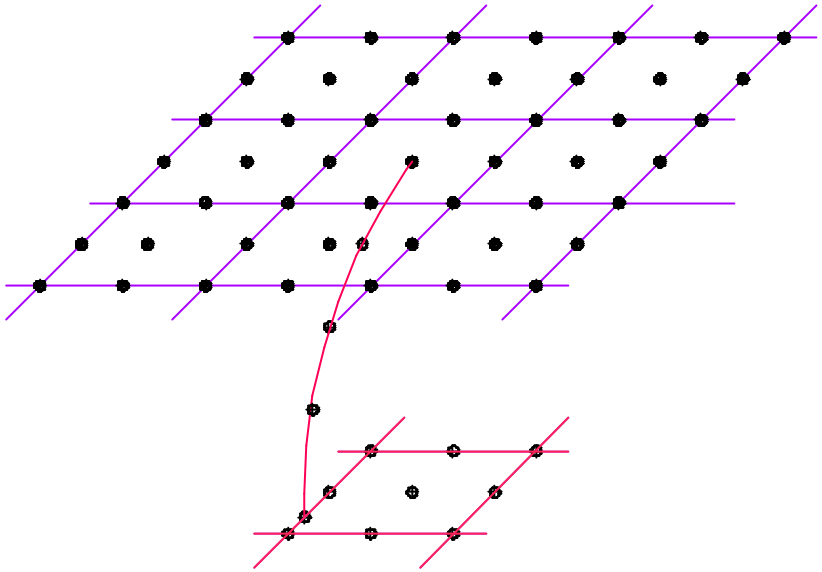
Approximation of energy equation

- Now it is convenient to implement finite element method since discrete L_2 – norm for η is natural for FEM.

- Here we again remove inertial terms out of variational formulation due to approximation along trajectories with defect correction and then we are able to implement traditional finite element method without any violations like upwind tricks and artificial viscosity.

- Among different types of finite elements we again take the same triquadratic finite elements on hexahedrons including curvilinear ones in the vicinity of body.

Again domains of approximation are different for inertial terms and the rest of them and can be taken the same for energy and all components of velocity



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Reduced energy equation at time level t

Due to trajectory method for inertial terms the equation became simpler for finite element implementation
at the time level t where Δt means temporal size:

$$\frac{\rho\eta}{\Delta t} - \frac{1}{\eta}\frac{\partial}{\partial x}\left(2\tilde{\mu}\eta\frac{\partial \eta}{\partial x}\right) - \frac{1}{\eta}\frac{\partial}{\partial y}\left(2\tilde{\mu}\eta\frac{\partial \eta}{\partial y}\right) + \frac{P}{\eta}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) - \frac{\Phi}{\eta} = f_e \tag{21}$$

Direct Navier-Stokes equations

- 1. At each time level the continuity equation is solved by approximation of differences along trajectories with defect correction iterations using smoothness almost along trajectories.

- 2. At each time level the momentum equations are firstly simplified due to approximation of inertial terms along trajectories. Then they are solved by triquadratic finite elements on hexahedrons including curvilinear elements for the better approximation of curvilinear boundaries.

- 3. The energy equation firstly transformed by substitution $\eta = e^{1/2}$. At each time level the transformed equation is simplified due to approximation of inertial terms along trajectories. Then it is solved by triquadratic finite elements on hexahedrons including curvilinear ones.

CPU + GPU

- MPI: Message passing interface
  - Language for data exchange
  - Local and shared clusters
- CUDA: Parallel computing architecture on graphics processing units
  - CUDA is a parallel computing architecture and technology that enables dramatic increases in computing performance by harnessing the power of the graphics processing units (GPU)

- Thank you for your attention!