Identification of vortices in flow using Graphics Processing Unit (GPU)

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Outline

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Overview of GPU computing

Identification of vortices in flow fields

Numerical results

Conclusion

Raise of GPU computing

- Graphics Processing Units (GPU) has evolved under pressure of computer games into very powerful though highly specialized chips with many cores used for *fast rendering of images* – pixels independent, single precision, specific datatypes
- early General-purpose computing on Graphics Processing Units (GPGPU) – difficult and marginal – but attract some attention on its performance – people realized, that they have (a certain type of) multicore chips already in their computers at the same time when CPU vendors anounced transition to two or four cores
- **June 2007** – milestone – NVIDIA released *Compute Unified Device Architecture* (CUDA) version 1.0 – a 'human-friendly' interface that presents an extension to C++

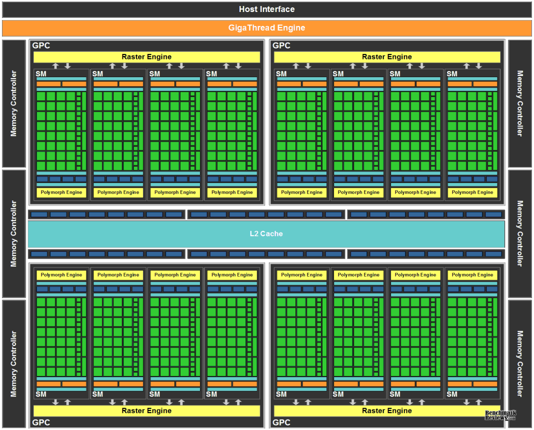
Raise of GPU computing

- December 2008 – *OpenCL* 1.0 released – standardization of GPU-type computing (Apple, NVIDIA, AMD, IBM, Intel, and others)
- March 2010 – release of Fermi type chips by NVIDIA
- November 2010 – in Top 500 list of most powerful computers (www.top500.org), Chinese computers *Tianhe-1A* and *Nebulae* ranked 1st and 3rd, respectively – both based on NVIDIA Tesla 2050/2070 cards for acceleration

CUDA

- Compute Unified Device Architecture
- NVIDIA's attempt to enter high performance computing (HPC)
- currently version 2.1
- extension to C++
- collection of driver, compiler, debugger, visual profiler and sample codes to provide basic tools for quick development of new applications

Fermi GPU chip



- 512 stream processors 700 MHz
- 1,536 MB RAM (GeForce 480), 15 streming multiprocessors
- GeForce (general use), Tesla (HPC), Quadro (CAD)
- 1,345 Gflops (CPU AMD Athlon X4 around 0.5 Gflops)

Memory hierarchy on GPU

NVIDIA GeForce GTX 480:

- device memory (1,536 MB) – bandwidth 177 GB/s
- shared memory (64 kB per multiprocessor) – bandwidth 1.344 TB/s
- texture memory
- registers

Efficient usage of memory levels is the key to exploit the GPU power.

Program execution on a GPU

- basic program unit is a *thread*
- 32 threads make a *warp* that is assigned to a multiprocessor – can synchronize, use shared memory to communicate data
- when executed, several warps are assigned to each multiprocessor and served by a sophisticated *runtime system*
- in CUDA code, threads are grouped into two dimensional *blocks* – for optimal performance, size of block is a multiple of size of the multiprocessor
- data divided into *blocks* which are executed by multiprocessors – single thread corresponds to single data unit (e.g. array element)
- *blocks* are organised into two dimensional *grid*

Program execution on a GPU

1. serial code running at CPU allocates space in memory of GPU and copies data to it (device memory)
2. parallel execution of *kernel function*
3. after completion, data are stored in memory of GPU and copied back to RAM, control is given back to CPU

Kernel function

- written for a single thread
- preferably accessing private memory location
- executed by runtime system

Sample kernel function

Function that copies integer 2D array x to y

```
__global__ void kernel_copy(int ldim, int *x, int *y)
{
 // where am I, from 0
 unsigned int i = blockIdx.x*blockDim.x+threadIdx.x;
 unsigned int j = blockIdx.y*blockDim.y+threadIdx.y;

 // copy my array
 y[i+ldim*j] = x[i+ldim*j];
}
```

The kernel is invoked by calling:

```
kernel_copy <<<dimGrid,dimBlock>>>(1, d_a, d_b );
```

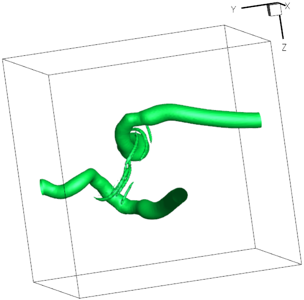
Here d_a and d_b are pointers to device memory.

Problems suitable for GPU computing

- **arithmetic intensity** – memory transfers slow, data should reside in device memory as long as possible with large operations/transfers ratio – **It is usually not straightforward to use GPU by a set of library functions!**
- low memory requirements for each thread
- low or no amount of communication among threads – access to non-local memory can slow down the computation
- no need for global synchronization of threads during kernel execution
- first GPU libraries are emerging – e.g. MAGMA project – linear algebra for GPU (group of Prof. Dongarra) – collaboration of CPU and GPU

Outline

Motivation



Interaction of Burgers vortices, DNS data by Prof. Rist (IAG Stuttgart)

- *visualization* of vortical structures in a flow is important in numerous areas of fluid mechanics, mainly in modelling of turbulence
- a generally accepted definition of *a vortex* and its identification in flow field is still missing
- existing methods for vortex identification are not general enough to cover all types of vortical flows

Basics of vortex identification

- current vortex identification methods are mostly based on double decomposition of velocity gradient matrix

$$\nabla \mathbf{u} = \mathbf{S} + \mathbf{\Omega},$$

where

  - $\mathbf{u} = (u, v, w)$ ... flow velocity
  - $\mathbf{S}$ ... *strain rate tensor*, $\mathbf{S} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$
  - $\mathbf{\Omega}$ ... *vorticity tensor*, $\mathbf{\Omega} = \frac{1}{2}(\nabla \mathbf{u} - (\nabla \mathbf{u})^T)$

This can be also written as

$$\mathbf{\Omega} = \frac{1}{2} \begin{pmatrix} 0 & -\omega_z & \omega_y \\ \omega_z & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{pmatrix},$$

where

$$\omega_x = \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}, \quad \omega_y = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}, \quad \omega_z = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$$

are components of *vorticity vector* $\omega = \nabla \times \mathbf{u}$.

Brief overview of existing methods

- popular methods are based on a definition of a scalar function that would locally discriminate vortex and non-vortex regions

chosen component of vorticity vector

- the simplest method
- plot ω_x, ω_y or ω_z according to known flow properties
- applicable only for known flow fields with vortical structures aligned with an axis

magnitude of vorticity vector

- defined as $|\omega|$
- invariant under rotation
- able to quantify the swirling motion
- influenced by shear

Brief overview of existing methods

Q-criterion [Hunt et al. (1988)]

- positive second invariant of ∇u
- region where vorticity magnitude dominates over strain-rate magnitude

$$Q = \frac{1}{2}\left(\|\boldsymbol{\Omega}\|^2 - \|\mathbf{S}\|^2\right) > 0$$

Here we use the norm $\|\mathbf{A}\|^2 = \mathrm{tr}(\mathbf{A}\mathbf{A}^T)$.

Brief overview of existing methods

Δ-criterion [Dallmann (1983), Vollmers et al. (1983), Chong et al. (1990)]

- define vortex as the region where ∇u has a pair of complex eigenvalues – this corresponds to spiral or closed streamlines
- for incompressible flows, this correspond to

$$\Delta = \left(\frac{Q}{3}\right)^3 + \left(\frac{R}{2}\right)^2 > 0,$$

where Q (see above) and $R = \mathrm{Det}(\nabla u)$ are invariants of ∇u.

Brief overview of existing methods

λ_2-criterion [Jeong and Hussain (1995)]

- dynamic considerations – search for *a pressure minimum across the vortex* – assumes that it corresponds with vortices
- define the vortex as a connected region, where the pressure Hessian, approximated by $\mathbf{S}^2 + \mathbf{\Omega}^2$, has two negative eigenvalues
- $\mathbf{S}^2 + \mathbf{\Omega}^2$ is symmetric – it has real eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3$
- the final criterion is thus defined as region where

$$\lambda_2 < 0$$

- valid for incompressible fluids only
- but the pressure minimum is neither sufficient nor necessary condition for existence of a vortex
- paper *On The Identification of a Vortex* has been cited about a thousand times (as for November 2010)

Triple Decomposition Method

- conventional double decomposition of motion near a point into symmetric and skew-symmetric parts corresponding to *straining motion* and *rigid rotation* has long history (Cauchy-Stokes decomposition theorem, 1845)
- both components are in general partially induced by *shear*
- *Triple Decomposition Method* (TDM) [Kolář (2007)] presents a novel approach to decompose relative motion near a point into **three** rather than two elementary components introducing *shear* besides *residual strain* and *residual rigid rotation*
- in TDM, velocity gradient tensor $\nabla \mathbf{u}$ is decomposed as

$$\nabla \mathbf{u} = \mathbf{S}_{RES} + \mathbf{\Omega}_{RES} + \nabla \mathbf{u}_{SH}$$

  where
  - $\mathbf{S}_{RES}$ ... residual strain tensor
  - $\mathbf{\Omega}_{RES}$ ... residual vorticity tensor
  - $\nabla \mathbf{u}_{SH}$ ... shear component

Principles of Triple Decomposition Method

The *pure shearing motion* is described by the *pure shear tensor* which appears in a suitable *reference frame* (i.e. under certain orthogonal transformations) as an *asymmetric matrix A*

$$a_{i,j} = 0 \text{ or } a_{j,i} = 0, i, j = 1, 2, 3.$$

- $\mathbf{S}_{RES} + \mathbf{\Omega}_{RES}$ form *residual tensor*,

$$\nabla \mathbf{u} = \begin{pmatrix} \text{residual} \\ \text{tensor} \end{pmatrix} + \begin{pmatrix} \text{shear} \\ \text{tensor} \end{pmatrix}$$

- the residual tensor consists of diagonal terms and symmetric or antisymmetric parts of the off-diagonal terms of $\nabla \mathbf{u}$, the 'leftovers' are moved to shear tensor

$$\begin{pmatrix} \text{res.} \\ \text{ten.} \end{pmatrix} = \begin{pmatrix} u_x & \operatorname{sgn}(u_y)\min(|u_y|, |v_x|) & \cdot \\ \operatorname{sgn}(v_x)\min(|u_y|, |v_x|) & v_y & \cdot \\ \cdot & \cdot & w_z \end{pmatrix}$$

- maximum of *effective shear* is extracted when norm of the *residual tensor* attains minimum

Example decomposition [Kolář (2007)]

$$\underbrace{\begin{pmatrix} -1 & 15 & 17 \\ 3 & 8 & -14 \\ -26 & -14 & -5 \end{pmatrix}}_{\nabla \mathbf{u}} = \underbrace{\begin{pmatrix} -1 & 3 & 17 \\ 3 & 8 & -14 \\ -17 & -14 & -5 \end{pmatrix}}_{residual\ \ tensor} + \underbrace{\begin{pmatrix} 0 & 12 & 0 \\ 0 & 0 & 0 \\ -9 & 0 & 0 \end{pmatrix}}_{\nabla \mathbf{u}_{SH}}$$

Triple Decomposition Method

- using standard strain-rate and vorticity tensors $\mathbf{S}$ and $\boldsymbol{\Omega}$, the following expression holds [Kolář (2007)]

$$||\nabla \mathbf{u}||^2 = \left|\left|\left(\begin{array}{c} \text{residual} \\ \text{tensor} \end{array} \right)\right|\right|^2 + 4(|S_{12}\Omega_{12}| + |S_{23}\Omega_{23}| + |S_{31}\Omega_{31}|).$$

- minimum of the residual tensor norm corresponds to the reference frame where maximum of the term

$$|S_{12}\Omega_{12}| + |S_{23}\Omega_{23}| + |S_{31}\Omega_{31}|$$

is attained.

Basic Reference Frame (BRF)

- the previously defined frame is called *basic reference frame (BRF)* and its determination can be stated as the problem: *Find orthogonal matrix* $\mathbf{Q}_{BRF}$ *such that*

$$\max_{\mathbf{Q}}(|S_{12}\Omega_{12}| + |S_{23}\Omega_{23}| + |S_{31}\Omega_{31}|) \tag{1}$$

  is attained, where

$$\begin{aligned} \mathbf{A} &= \mathbf{Q}(\nabla\mathbf{u})\mathbf{Q}^T, \\ \mathbf{S} &= \frac{1}{2}\left(\mathbf{A} + \mathbf{A}^T\right), \\ \mathbf{\Omega} &= \frac{1}{2}\left(\mathbf{A} - \mathbf{A}^T\right). \end{aligned}$$

- in this optimization problem, $\mathbf{Q}$ is constructed from three angles of rotating frame along axes, $Q = f(\alpha, \beta, \gamma)$, $0 \le \alpha < \pi$, $0 \le \beta < \pi$, $0 \le \gamma \le \pi/2$

Basic Reference Frame (BRF)

- BRF is in general different and independent for each point of the flow field – whole range of angles must be taken into account at every position when looking for it
- to find BRF numerically, ranges of angles are uniformly discretized with reasonable (angle) step size and the expression (1) is evaluated for combinations of α_i, β_j and γ_k
- while finer step size allows better localization of the BRF, it results in increase of required objective function evaluations since there is $1/\Delta\alpha^3$ dependence on the step size $\Delta\alpha$ (e.g. 2,981,251 evaluations for step size 1 deg)

TDM for vortex identification

Once approximation to $\mathbf{Q}_{BRF}$ is known, we determine the residual vorticity by

1. transform the velocity gradient into BRF by

$$\mathbf{A} = \mathbf{Q}_{BRF}(\nabla\mathbf{u})\mathbf{Q}_{BRF}^{T},$$

2. get residual tensor $\mathbf{A}_{RES}$ from $\mathbf{A}$
3. perform double decomposition to obtain *residual* strain-rate tensor $\mathbf{S}_{RES}$ and *residual* vorticity tensor $\mathbf{\Omega}_{RES}$

$$\begin{aligned}\mathbf{S}_{RES} &= \frac{1}{2}\left(\mathbf{A}_{RES} + \mathbf{A}_{RES}^{T}\right),\\ \mathbf{\Omega}_{RES} &= \frac{1}{2}\left(\mathbf{A}_{RES} - \mathbf{A}_{RES}^{T}\right).\end{aligned}$$

4. a *vortex* is defined as a connected region where $\|\mathbf{\Omega}_{RES}\| > 0$

- TDM eliminates the effect of shear on vorticity
- capable of describing a vortex in incompressible as well as compressible fluids

TDM in 2D

In 2D – vortex axis is always peripendicular to flow plane – the method simplifies due to one axis of BRF set perpendicular to the plane to the following formulas:

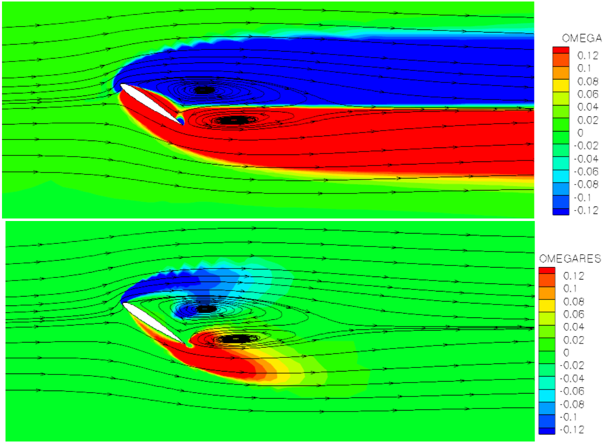
$$\omega_{RES} = \begin{cases} 0 & \text{for} \quad |s| \geq |\omega| \\ \mathrm{sgn}(\omega)(|\omega| - |s|) & \text{for} \quad |s| \leq |\omega| \end{cases} ,$$

where e.g. for incompressible flow

$$\begin{aligned} |s| &= \left(\sqrt{4\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2} \right) /2, \\ \omega &= \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) /2. \end{aligned}$$

Outline

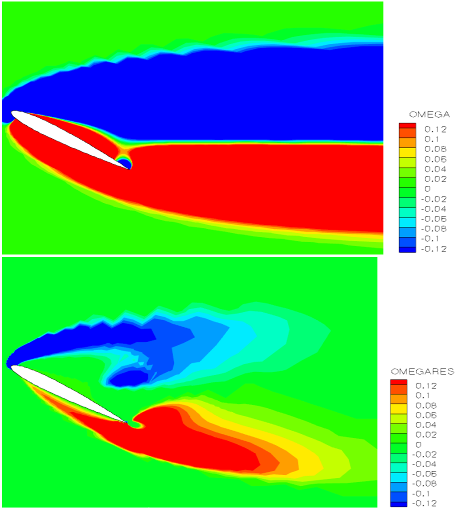
Numerical example in 2D



Vorticity defined by 'standard' two-dimensional vorticity tensor component ω (top) and by *residual vorticity* (bottom) in flow past NACA 0012 airfoil, $\alpha = 34^\circ$, Re $= 100$

FEM data by Dr. Jaroslav Novotný

Numerical example in 2D

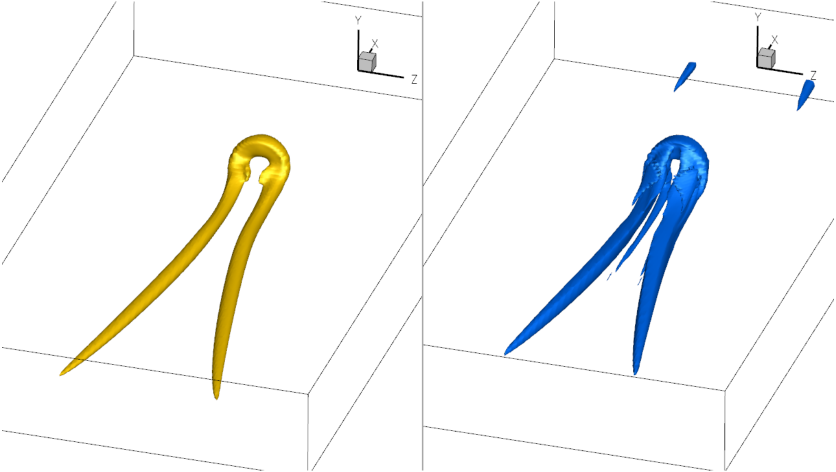


Details of vorticity defined by 'standard' two-dimensional vorticity tensor component ω (top) and by *residual vorticity* (bottom) in flow past NACA 0012 airfoil, $\alpha = 34^\circ$, Re $= 100$

Numerical example in 3D

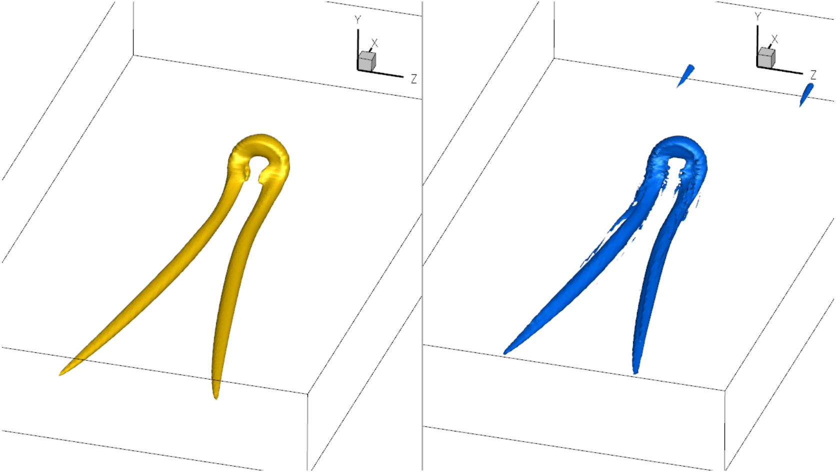
- in 2D, TDM is very competitive, in 3D it poses a practical issue of computational costs due to the neccessity of finding the BRF, experiments have shown that in general cases the choice of step of angles may have a large impact on the quality of the identification and thus the step size of 1-10 degrees is recommended
- BRF is specific for each data point – 2,981,251 possibilities for step size 1 deg
- BRF for each point is independent – presents an *embarassingly parallel* computation – specific properties of GPU can be exploited to speed-up calculations
- flow data for 3D DNS simulations are due to kindness of the team of Prof. Rist from IAG Stuttgart

Numerical example in 3D



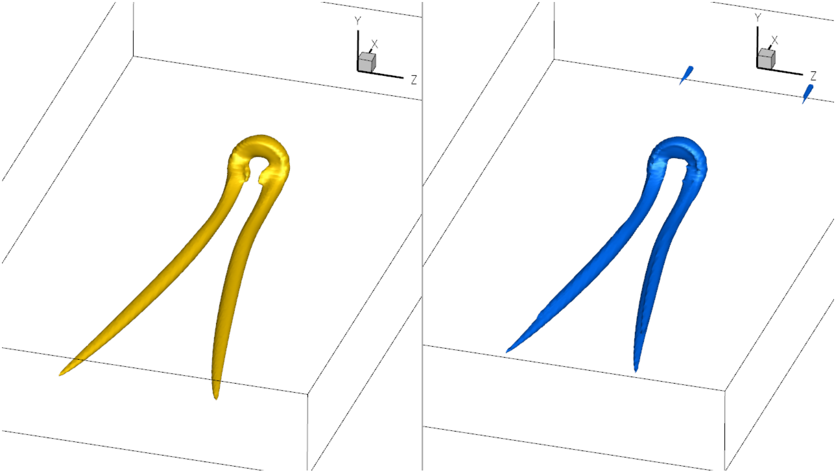
Ω-vortex in boundary layer, comparison of λ_2-method at 4.6% treshold (left) and residual vorticity at 13% treshold, BRF search step 90 deg (right)

Numerical example in 3D



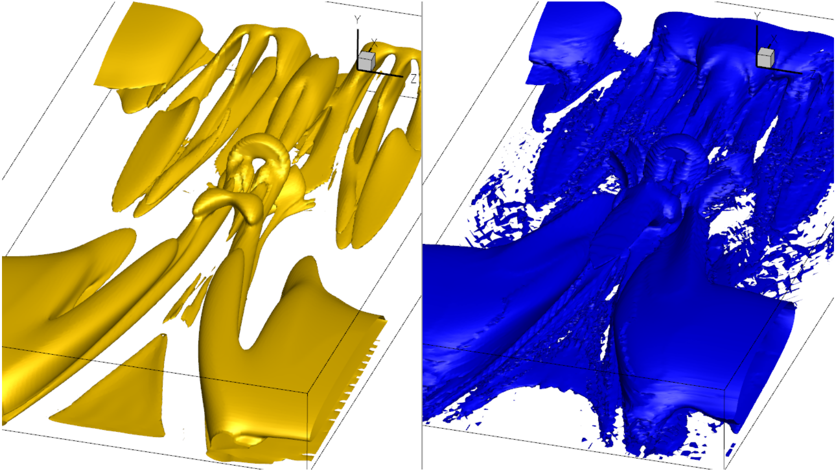
Ω-vortex in boundary layer, comparison of λ_2-method at 4.6% treshold (left) and residual vorticity at 13% treshold, BRF search step 30 deg (right)

Numerical example in 3D



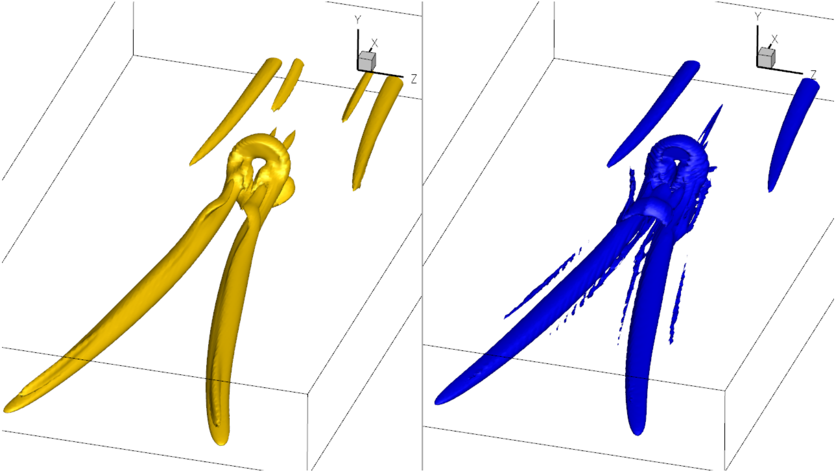
Ω-vortex in boundary layer, comparison of λ_2-method at 4.6% treshold (left) and residual vorticity at 13% treshold, BRF search step 1 deg (right)

Numerical example in 3D



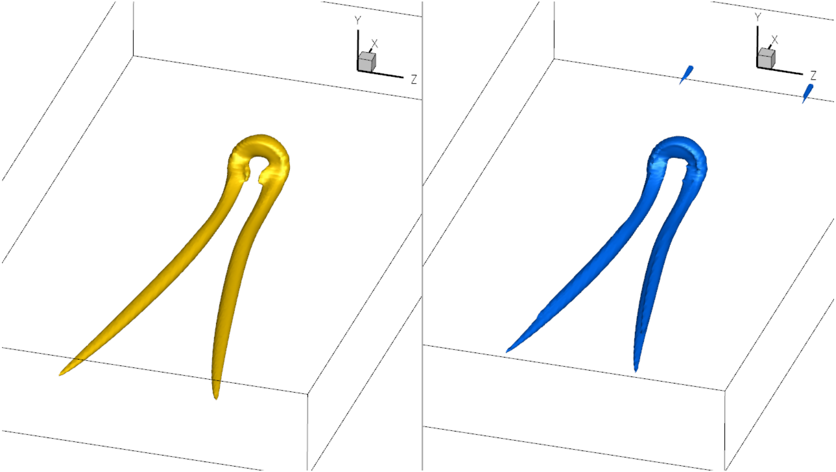
Ω-vortex in boundary layer, comparison of λ_2-method at 0.03% treshold (left) and residual vorticity at 0.2% treshold, BRF search step 1 deg (right)

Numerical example in 3D



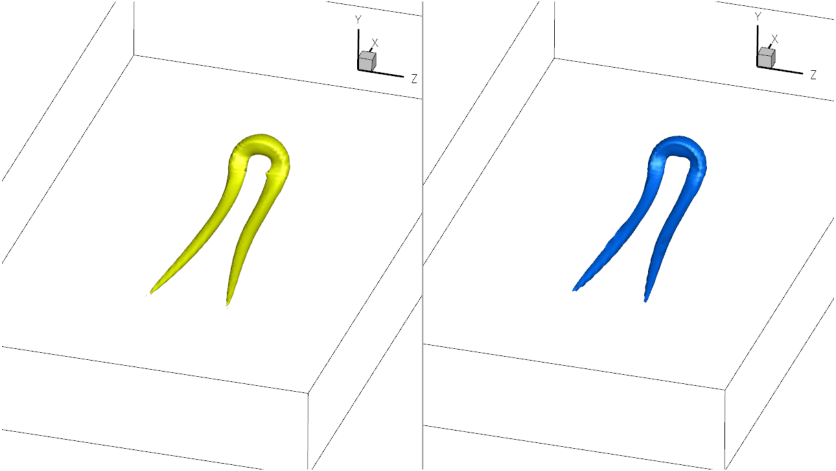
Ω-vortex in boundary layer, comparison of λ_2-method at 0.76% treshold (left) and residual vorticity at 2.2% treshold, BRF search step 1 deg (right)

Numerical example in 3D



Ω-vortex in boundary layer, comparison of λ_2-method at 4.6% treshold (left) and residual vorticity at 13% treshold, BRF search step 1 deg (right)

Numerical example in 3D



Ω-vortex in boundary layer, comparison of λ_2-method at 7.6% treshold (left) and residual vorticity at 19.4% treshold, BRF search step 1 deg (right)

Computational times

step	import (s)	BRF (s)		$\|\Omega\|_{RES}$	λ_2 (s)
		GF 9650M GT	GTX 480		
90	15.6	0.4	0.05	1.4	4.9
45		2.0	0.13		
30		6.7	0.34		
10		172.8	8.0		
5		1,373.1	63.9		
2		4,093.7	997.8		
1		n/a	2,220.6		

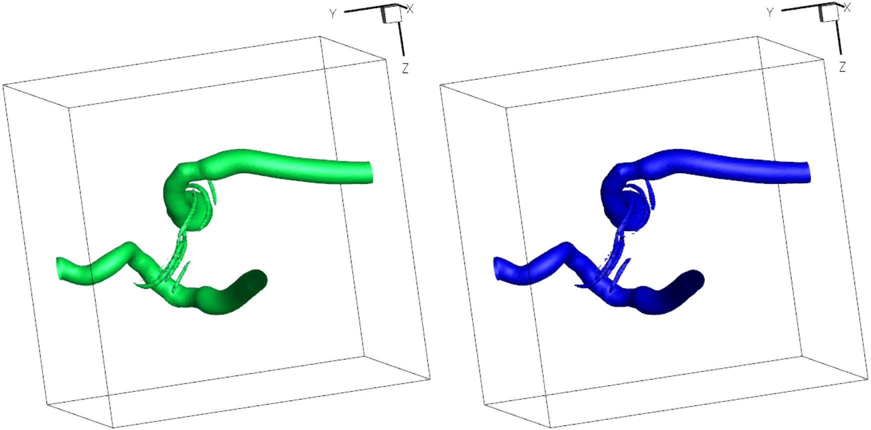
- GF 9650M GT ... NVIDIA GeForce 9650M GT (my laptop)
- GTX 480 ... NVIDIA GeForce GTX 480 (recently acquired by Institute of Mathematics)
- computational times on Tesla T10 GPU (UC Denver) comparable to GTX 480

Computational times

Serial computation of BRF on laptop CPU (Intel Core Duo 2.53 GHz):

- for step size 2 deg, one point takes 142 ms
- the problem presented consists of $175 \times 101 \times 129 = 2{,}280{,}075$ points
- the serial computation would take about 90 hours on CPU of my laptop
- it would take about **28 days** with step size 1 deg

Numerical example in 3D



Burgers vortex, Ma $= 0.3$, comparison of λ_2-method at 3.9% treshold (left) and residual vorticity at 16% treshold, BRF search step 1 deg (right)

Outline

Conclusion

- Triple Decomposition Method (TDM) appears to be competitive with standard vortex identification methods in terms of quality of vortex identification
- TDM may be costly procedure for fine resolution
- it offers a good intuitive insight into the process of vortex identification
- the method is subject to ongoing research and some related methods are being developed [Kolář, Moses, Šístek (2010)]
- determination of basic reference frame is a 'dream problem' to be addressed by GPU computing
- achieved speed-up 80 (within a laptop) or 340 (on the new generation GPU chip) made from the TDM method
  a candidate for fine analysis of vortical structures in a complex flow field
- code *Vortex Analyzer* available to public at my website `http://www.math.cas.cz/~sistek`

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References

[1] Jeong, J., Hussain, F.: On the identification of a vortex. J. Fluid Mech. **285**, 69-94 (1995)

[2] Kolář, V.: Vortex identification: new requirements and limitations. Int. J. Heat Fluid Flow **28**(4), 638 - 652 (2007)

[3] Kolář, V., Moses, P., Šístek, J.: Local corotation of line segments and vortex identification. In: Mallinson, G. and Cater, J. (eds.) Proceedings of the 17th Australasian Fluid Mechanics Conference, Auckland, New Zealand, 2010.

[4] Kolář, V., Moses, P., Šístek, J.: Triple Decomposition Method for Vortex Identification in Two-Dimensional and Three-Dimensional Flows, To appear in *Computational Fluid Dynamics 2010*, Proceedings of The 6th ICCFD Conference, St. Petersburg, Russia, July 12–16, 2010.