COMPUTATIONAL MECHANICS: *A POWERFUL SCIENTIFIC METHODOLOGY*

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Talk presented at

Super Computer Annual User Meeting - 6 May 2009

20^{th} Anniversary Celebration

GENERAL REMARKS

One of the most important things engineers and scientists do is to *model* physical phenomena

(1) Conduct physical experiments

(2) Develop mathematical models

(3) Numerically simulate them

(4) Design systems

(5) Manufacture systems

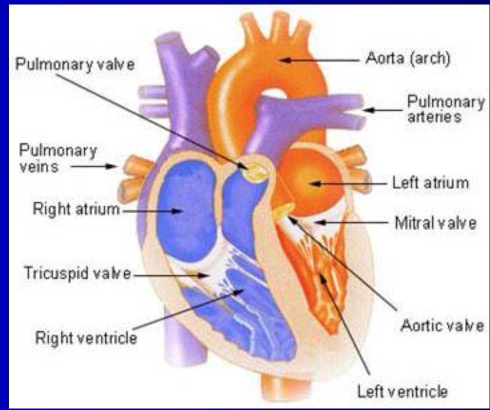
CURRENT DEVELOPMENTS

- Numerical simulations of new systems
- Enhancement/refinement of existing element technologies
- Development of novel computational frameworks

Overall Objective

- Multiscale modeling of complex biological cells and tissues
- Apply knowledge for the development of new diagnostic & treatment tools and prosthetics

Temporal Scale



Mechanics of Organs

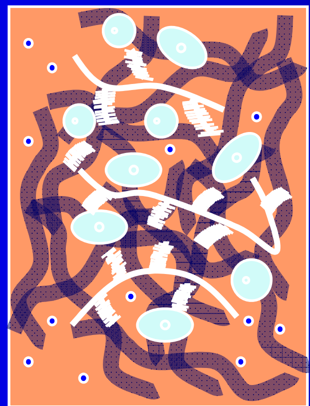
Diagnosis and Treatment

DISEASES

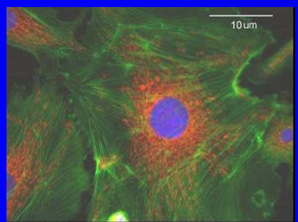
Breast Tumor
Cancer cell
Cardiovascular Diseases

SCAFFOLDS

Skin graft
Vascular tissue



Mechanics of Tissues



Mechanics of Cell

Spatial Scale

Nano–Micro Scale | Micro-Meso Scale | Meso-Macro Scale

Nonlinear Shell Theory

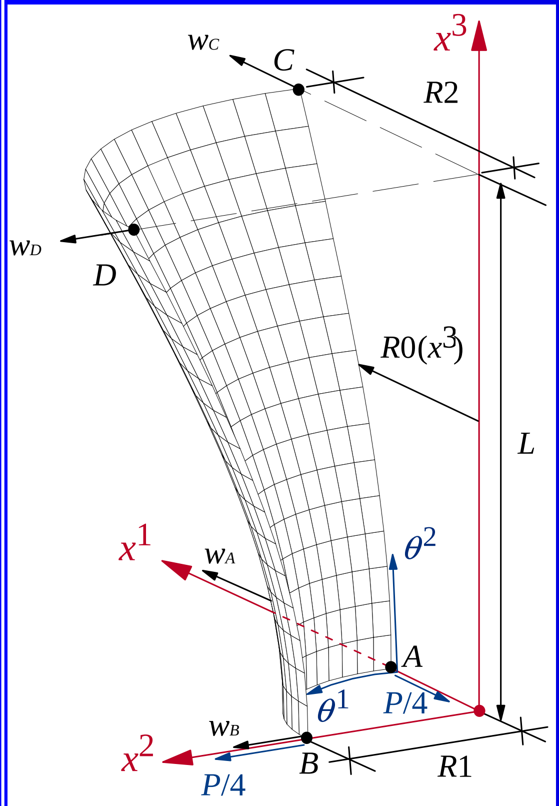
The displacement field:

$$\mathbf{v}\left(\theta^{i}\right)=\mathbf{u}\left(\theta^{\alpha}\right)+\theta^{3}\boldsymbol{\varphi}\left(\theta^{\alpha}\right)+(\theta^{3})^{2}\underline{\boldsymbol{\psi}}\left(\theta^{\alpha}\right)$$

Seven kinematic variables $\left(u_i,\varphi_i,\psi_3\right)$

- Refined shell theory that accounts for transverse shear deformation and thickness change is developed
- Use a hyperelastic constitutive model, and assume linear relation between **S** and **E**.

Composite hyperboloidal composite shell



$$E_1 = 40.0 \times 10^6,\ E_2 = E_3 = 1.0 \times 10^6$$

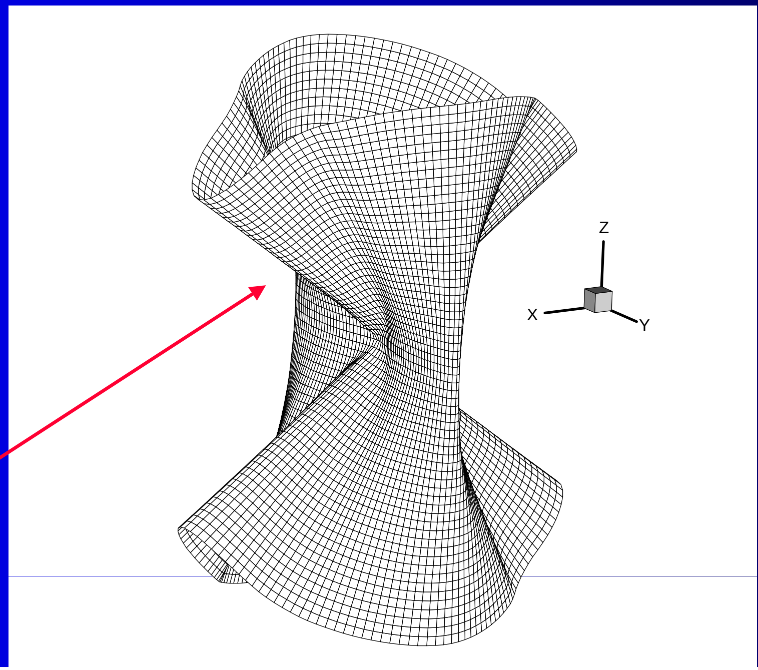
$$G_{12} = G_{13} = G_{23} = 0.6 \times 10^6$$

$$C = 20/\sqrt{3}$$

$$\nu_{12} = \nu_{13} = \nu_{23} = 0.25$$

$$R_1 = 7.5,\ R_2 = 15.0,\ L = 20.0,\ h = 0.04$$

$$R_0\left(x^3\right) = R_1\sqrt{1 + (x^3/C)^2}$$



Deformed configuration

Hyperboloid

Desirable Features of a Computational Approach

- **Must preserve all features of the mathematical model in the formulation and associated computational model.**
- **Must be based on a formulation that seeks to minimize (in some meaningful sense) the error introduced in the governing equations.**
- **Avoid ad-hoc approaches to `fix' numerical deficiencies of the computational model.**

Currently Used Computational Schemes

- FEM in structural mechanics is based on minimum (energy) principles.
- FEM in fluid mechanics is based on weak forms (integral statements) of governing equations, and they are not equivalent to any minimum principle.
- FDM has no minimum principle in any field; they are based on truncated Taylor's series expansions of the derivatives in governing differential equations.

LEAST-SQUARES FINITE ELEMENT MODELS – BASIC IDEA

$$-\nabla^2 u = f \quad \text{in} \quad \Omega$$

$$(-\nabla^2 = -\nabla \cdot \nabla)$$

$$u = \hat{u} \quad \text{on} \quad \Gamma_u$$

$$\frac{\partial u}{\partial n} = \hat{g} \quad \text{on} \quad \Gamma_g$$

$$\mathbf{v} - \nabla u = 0 \quad \text{in} \quad \Omega$$

$$-\nabla \cdot \mathbf{v} = f \quad \text{in} \quad \Omega$$

$$u = \hat{u} \quad \text{on} \quad \Gamma_u$$

$$\hat{\mathbf{n}} \cdot \mathbf{v} = \hat{g} \quad \text{on} \quad \Gamma_g$$

$$\mathrm{I_m}(u, \mathbf{v}) = \| \mathbf{v} - \nabla u \|_{0,\Omega}^2 + \| -\nabla \cdot \mathbf{v} - f \|_{0,\Omega}^2 + \| \hat{\mathbf{n}} \cdot \mathbf{v} - \hat{g} \|_{0,\Gamma_g}^2$$

Minimize $\mathrm{I_m}$**:** $\delta \mathrm{I_m} = 0$ gives

$$\mathrm{B_m}((u, \mathbf{v}), (\delta u, \delta \mathbf{v})) = l_{\mathrm{m}}((\delta u, \delta \mathbf{v}))$$

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Example (using LSFEM Model 2):

Differential Equation

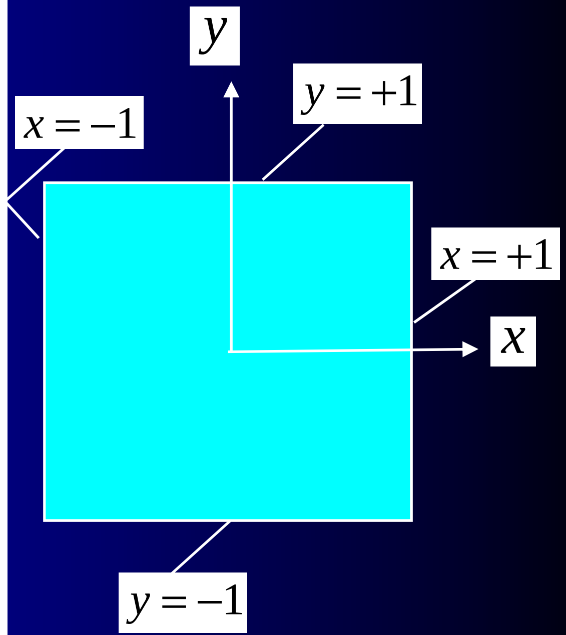
$$-\nabla^2 u = f \ \textbf{in} \ \textbf{-1} \le x, y \le \textbf{1}$$

Boundary Conditions

$$\frac{\partial u}{\partial y} \equiv v = 0 \ \text{on} \ y = \pm 1$$

$$\frac{\partial u}{\partial x} \equiv w = q^*(y) = 0 \ \text{on} \ x = -1$$

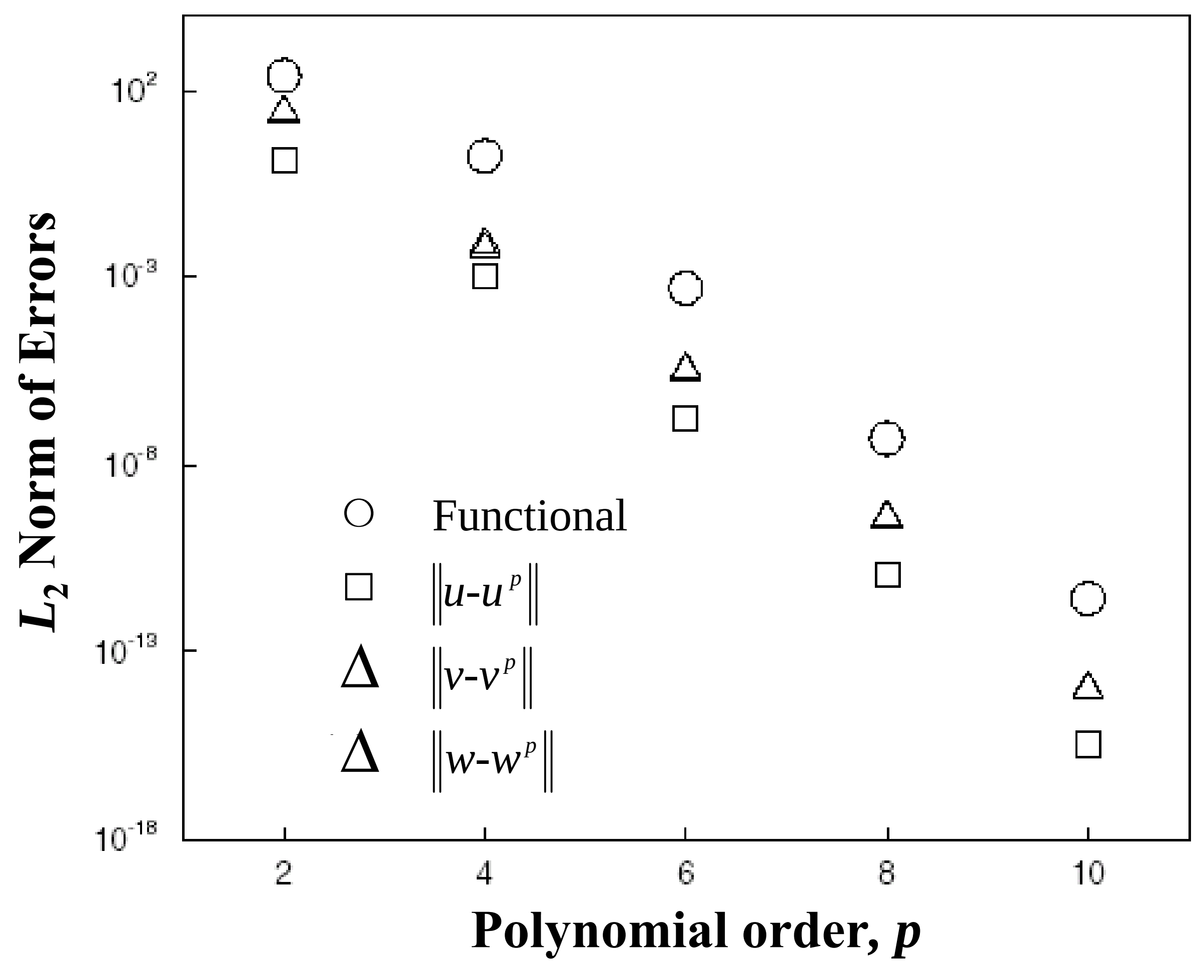
$$u = u^*(y) = 8\cos \pi y \ \text{on} \ x = 1$$



Analytical solution:

$$u(x, y) = (7x + x^7)\cos \pi y$$

Plots of the L_2-Error norms as a function of p



Velocity-pressure-vorticity Formulation

$$(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p-\frac{1}{\mathrm{Re}}\nabla\times\boldsymbol{\omega}=\mathbf{f}\quad \text{in}\quad \Omega$$

$$\boldsymbol{\omega}-\nabla\times\mathbf{u}=\mathbf{0}\quad \text{in}\quad \Omega$$

$$\nabla\cdot\mathbf{u}=0\quad \text{in}\quad \Omega$$

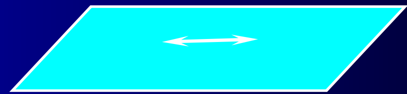
$$\nabla\cdot\boldsymbol{\omega}=0\quad \text{in}\quad \Omega$$

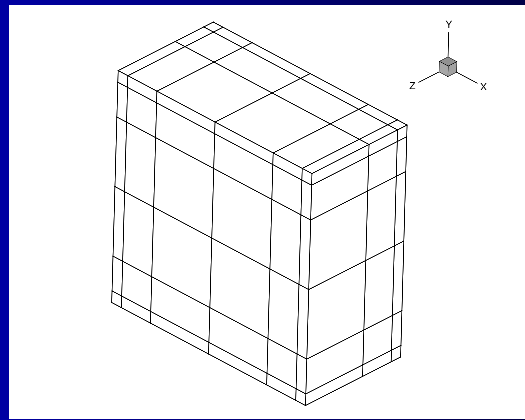
$$\mathbf{u}=\hat{\mathbf{u}}\quad \text{on}\quad \Gamma_{\mathrm{u}}$$

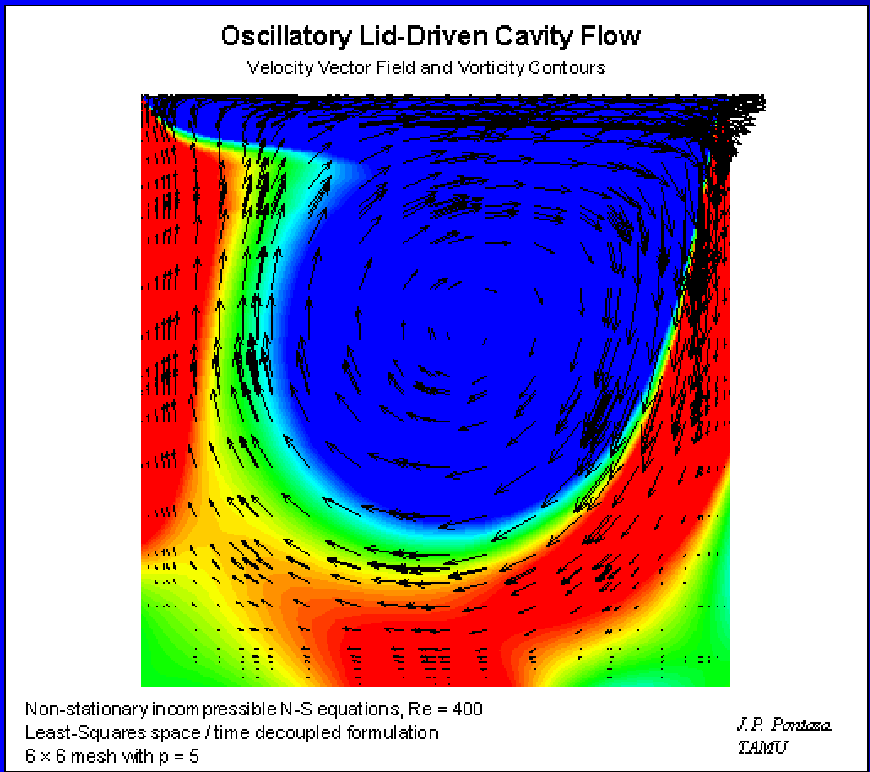
$$\boldsymbol{\omega}=\hat{\boldsymbol{\omega}}\quad \text{on}\quad \Gamma_{\omega}$$

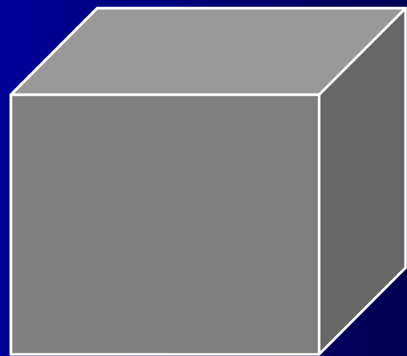
$$\mathcal{J}(\mathbf{u},p,\omega;\mathbf{f})=\frac{1}{2}\Big(\|(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p+\frac{1}{\mathrm{Re}}\nabla\times\omega-\mathbf{f}\|_0^2+\|\omega-\nabla\times\mathbf{u}\|_0^2 + \|\nabla\cdot\mathbf{u}\|_0^2+\|\nabla\cdot\omega\|_0^2\Big) \tag{27}$$

Oscillatory Flow of a Viscous Incompressible Fluid in a Lid-driven Cavity

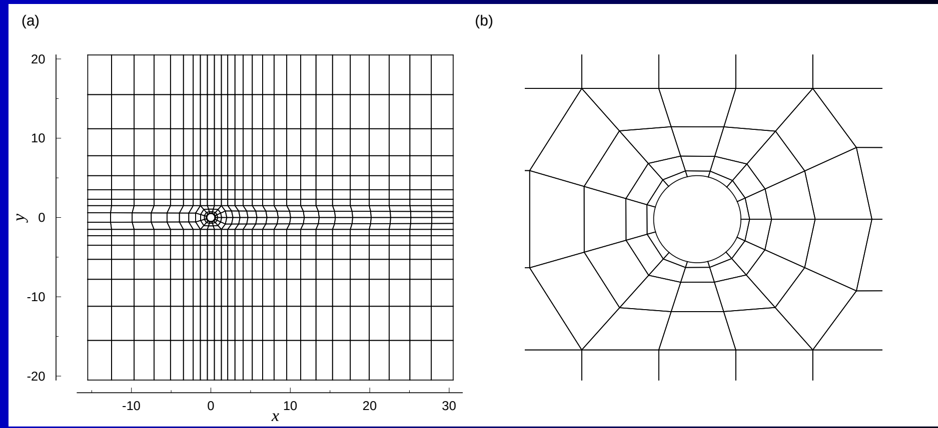






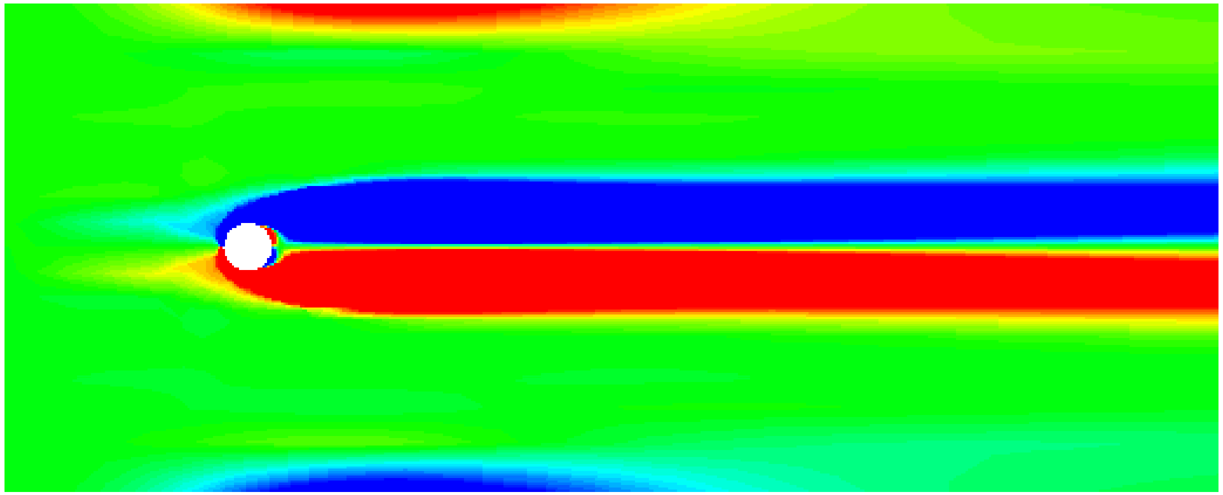


Flow of a Viscous Incompressible Fluid past a Cylinder



Circular Cylinder in Crossflow

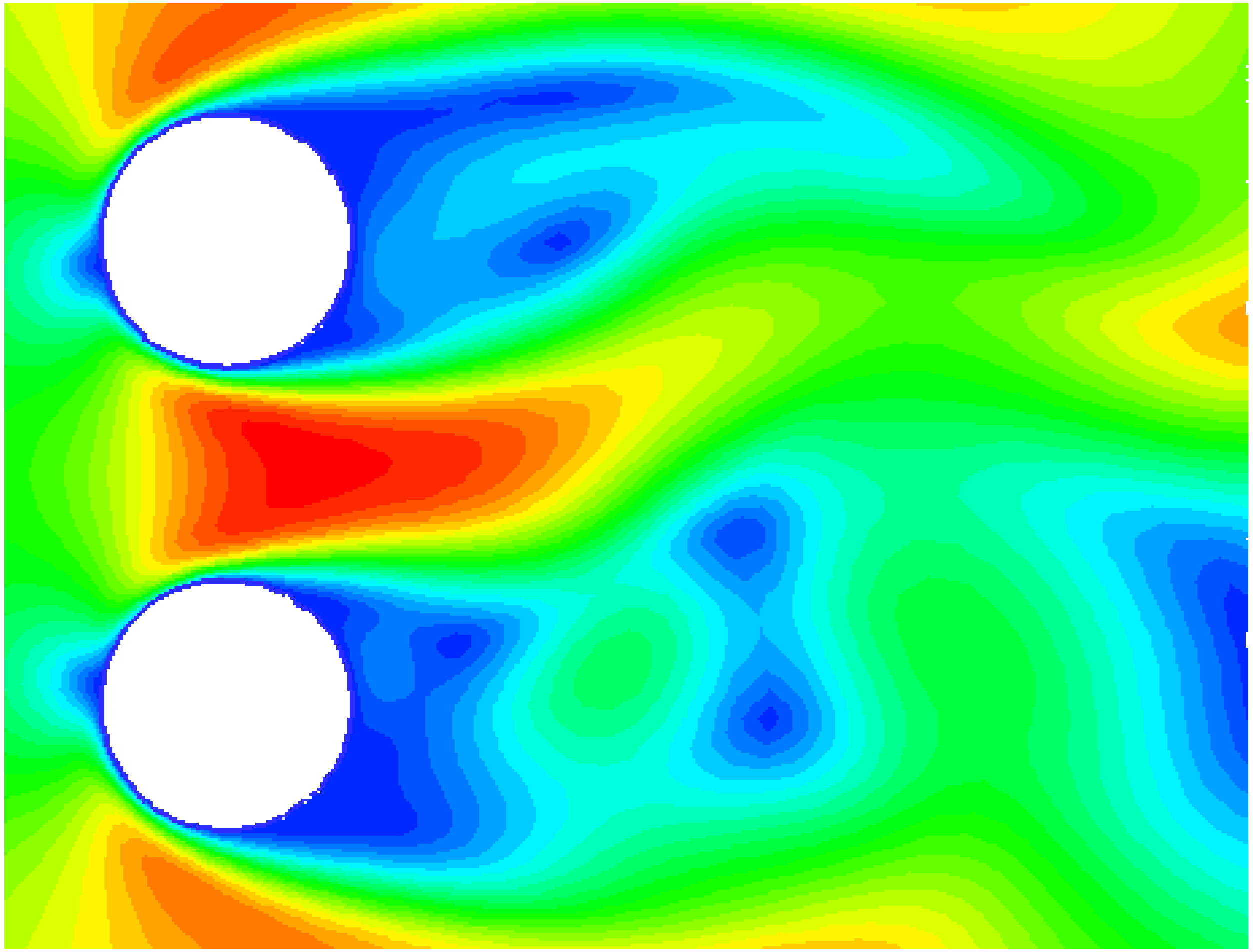
Vorticity Contours



Non-stationary incompressible N-S equations, Re = 100
Least-Squares time / space decoupled formulation
1200 elements with p = 2

J.P. Pontaza
TAMU

Incompressible flow past two circular cylinders in a side-by-side arrangement
surface-to-surface gap, S/D=0.85 , Re=100
velocity magnitude contours showing the "bistable gap jet" **300.000**



Least-squares finite element formulation
p-levels of 4/4/2 in space-time

J.P. Pontaza, 2004

CHALLENGES & OPPORTUINITIES

- **Material modeling at different scales presents new challenges in developing more sophisticated and accurate computational techniques.**
- **Constitutive models of new and multifunctional materials (nano-composites; biological materials; micromechanics and mesomechanics studies)**
- **Novel computational procedures for multi-physics and multi-scale modeling**

Acknowledgements to my students

I thank you (attendees)
for your interest
in my lecture

I thank Greta Thomas, and Richard (Lee) Panetta for their help and support with the super computer accounts for me and my students

That which is not given is lost