Institute of Fundamental Technological Research,
Polish Academy of Sciences (IPPT PAN)
Warsaw, 5th December 2007

Multi-Scale Simulations of Coupled Fluid Flow and Electromagnetism: From Origins of Planetary Magnetic Fields to Improved Cancer Therapy

S. Kenjeres*

Department of Multi Scale Physics and J.M. Burgers Centre for Fluid Mechanics
Faculty of Applied Sciences, Delft University of Technology

*** Royal Netherlands Academy of Arts and Sciences (KNAW) research fellow (2001-2006)**

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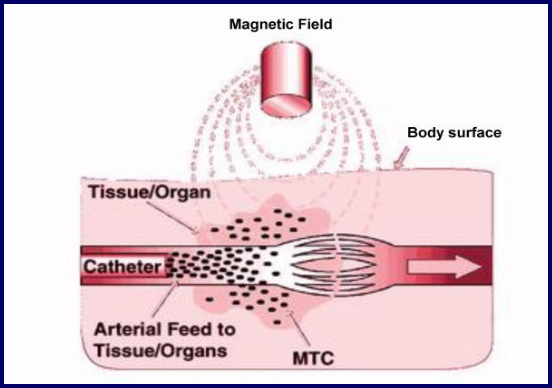
-MagnetoHydrodynamics (MHD):
electrically conductive fluid flow/electromagnetic fields interactions

-MHD interactions play the key role in many physical phenomena:

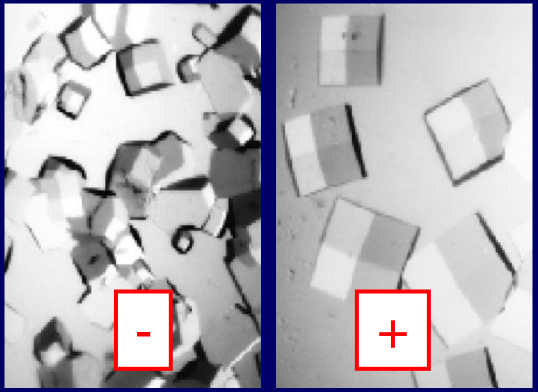
Continuous steel-casting

Aluminium reduction cells

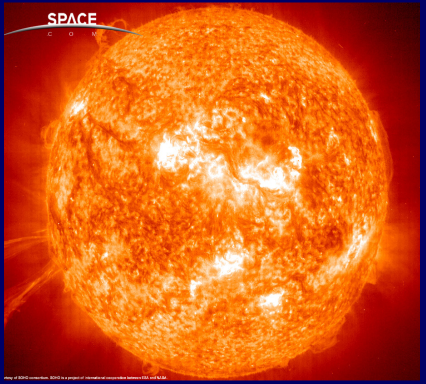
Magnetic Drug Delivery



Crystal growth

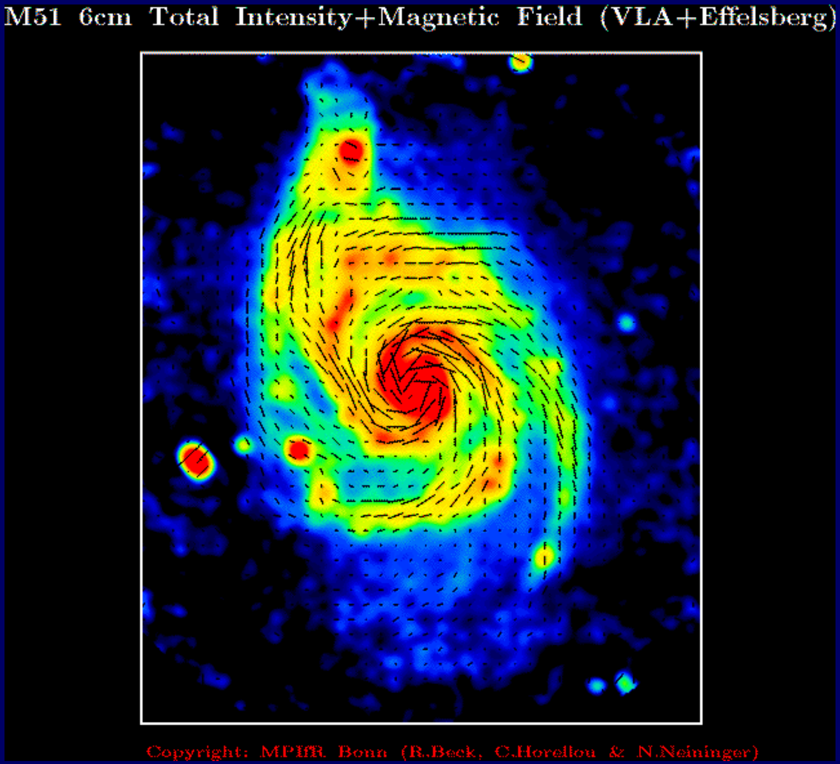


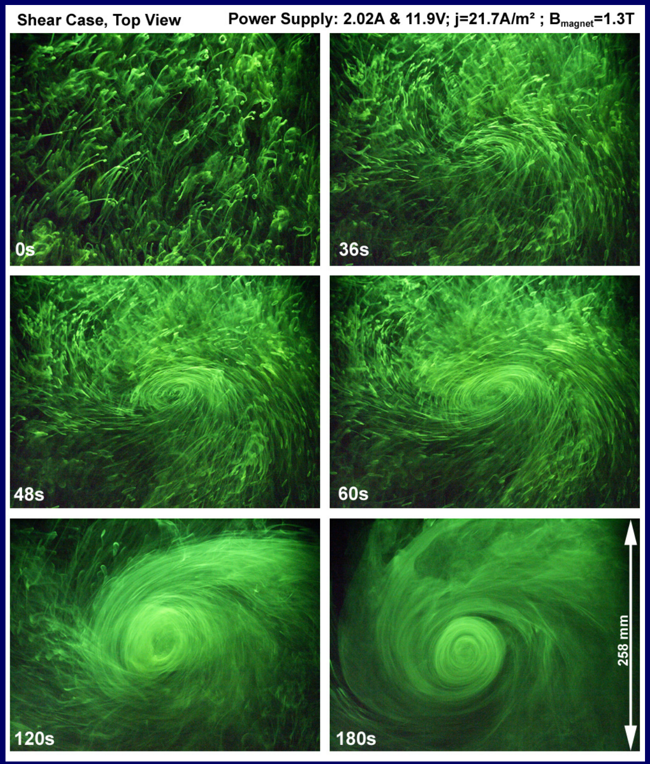
Geo- and Astro-physics



Magnetic Field: off – on

-Immense variety of scales:
from spiral galaxies to electro-magnetically driven mini tornados





-astronomical observations:

background magnetic field inside M51 galaxy, Beck *et al.* (2000)

-laboratory observations:

PLIF and PIV measurements, Verdoold *et al.* (2004)

2 permanent magnets + 2 electrodes

(perpendicular to each other)

Characteristic Dimensionless MHD Parameters

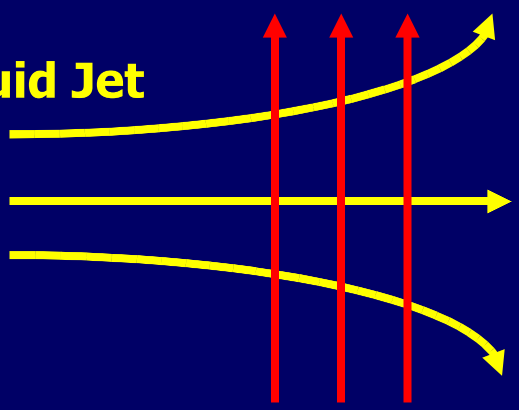
Reynolds number $Re = \dfrac{U \cdot D}{\nu}$ **Inertia/Viscous forces**

Magnetic Reynolds number $Re_m = \dfrac{t_d}{t_k} = \dfrac{\mu_0 \sigma D^2}{D/U} = \mu_0 \sigma U D$ **Stretching/Resistive dumping**

-Magnetic Dynamo:

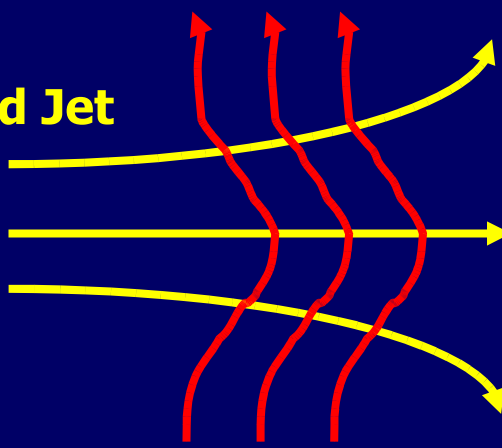
the process of partial conversion of the mechanical energy of a moving electrically conductive medium into the magnetic energy!

Fluid Jet



Magnetic Field **Re_m<<1**

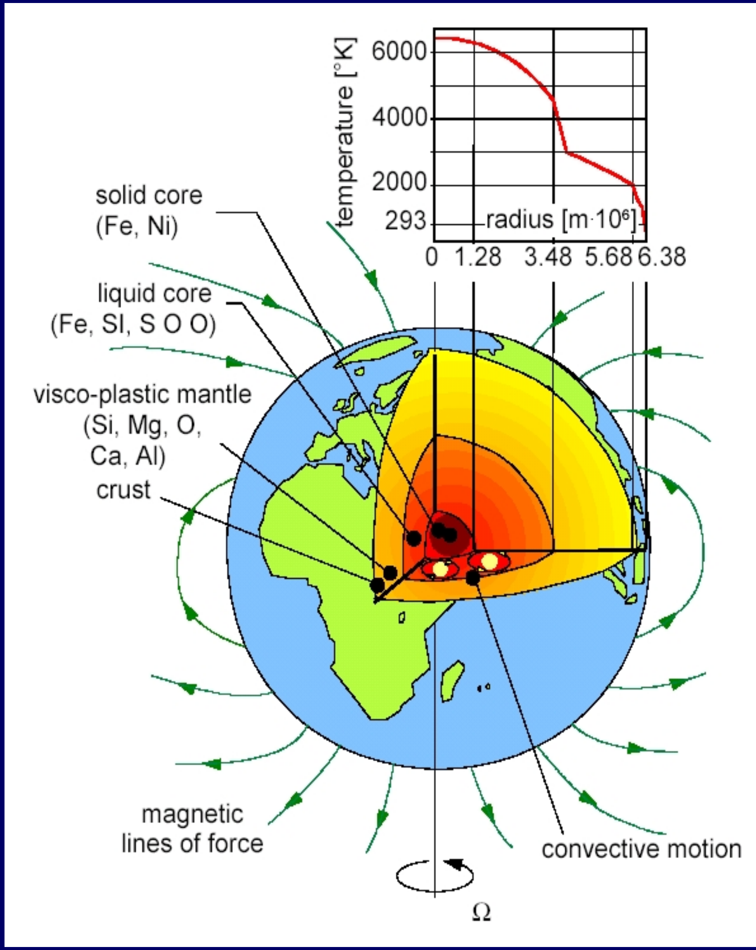
Fluid Jet



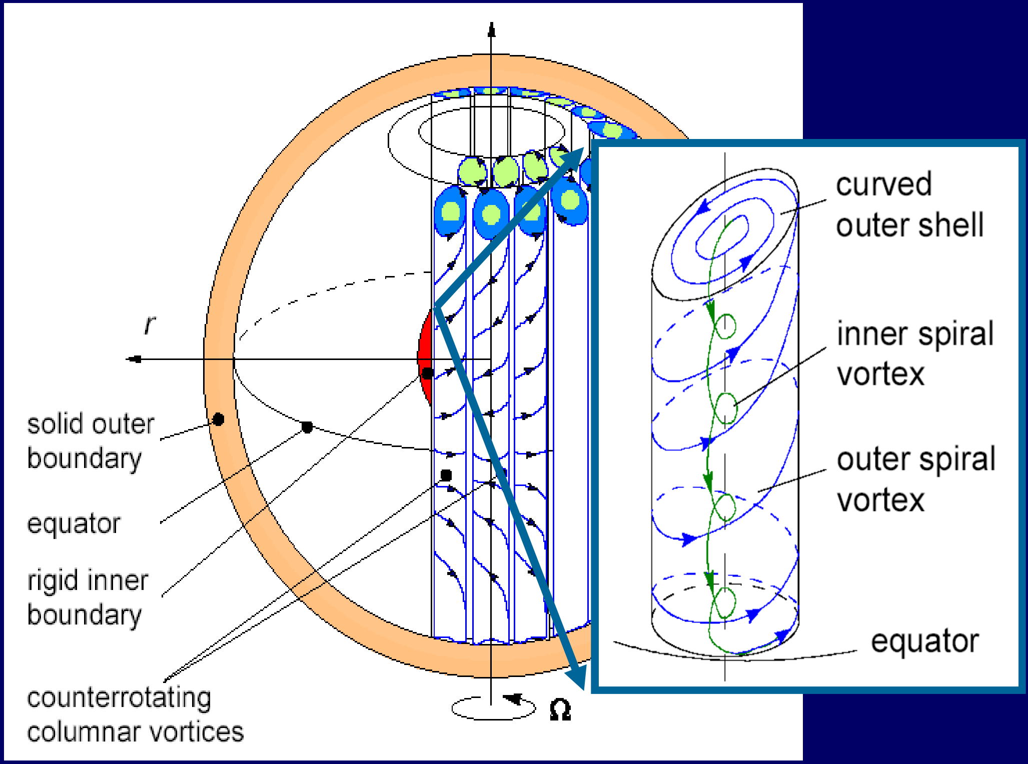
Re_m>1 **Magnetic Field**

Magnetic-Dynamo Condition: $Re_m > 1$!

Dynamo principle demonstration: geo-dynamo theory



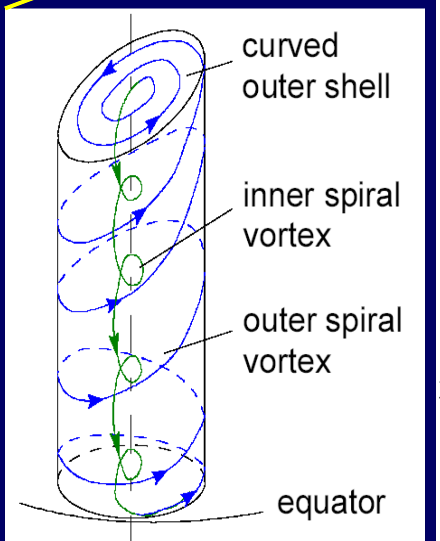
-Structure of the Earth,
Beatty and Chaikin (1990)

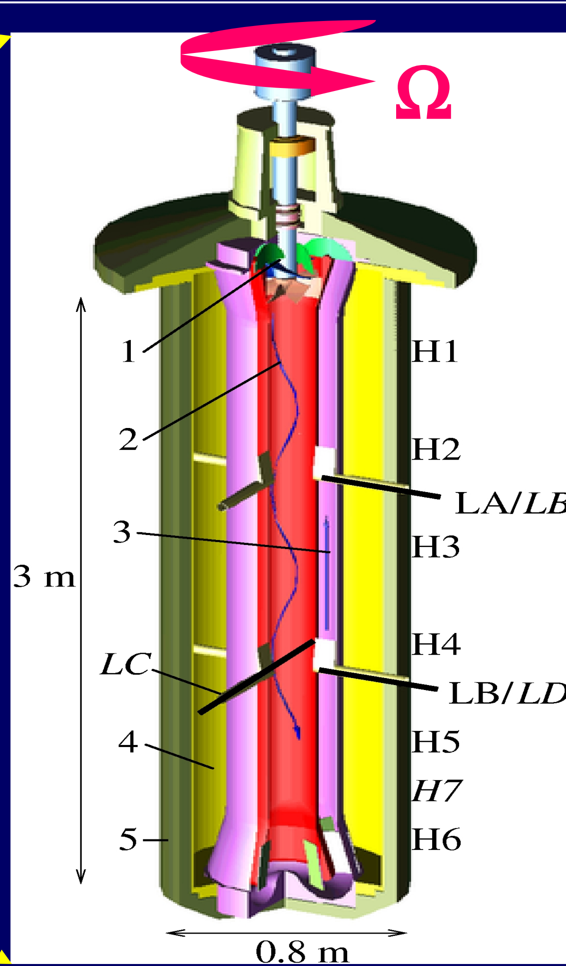


-Columnar vortex pattern of convection in
rotating sphere, Busse (1994)

Laboratory studies based on the Riga dynamo facilities

Gailitis *et al.* (1967,...,2004), Institute of Physics, University of Latvia





1. **Impeller**
2. **Helical flow region**
3. **Back-flow region**
4. **Sodium at rest**
5. **Stainless steel container**

H1…H7 – Hall probe sensors

$Re=3.5\times10^6$

$Re_m=10\text{-}30$

$Pr_m=6.5\times10^{-6}$

Sodium at 150°C, pump with 2x110 kW power !!

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Momentum + Magnetic Induction → Continuum Unifying Principles

$$\ldots \quad F_i^R = 2\varepsilon_{ijk} U_j \Omega_k \qquad F_i^L = \varepsilon_{ijk} J_j B_k$$

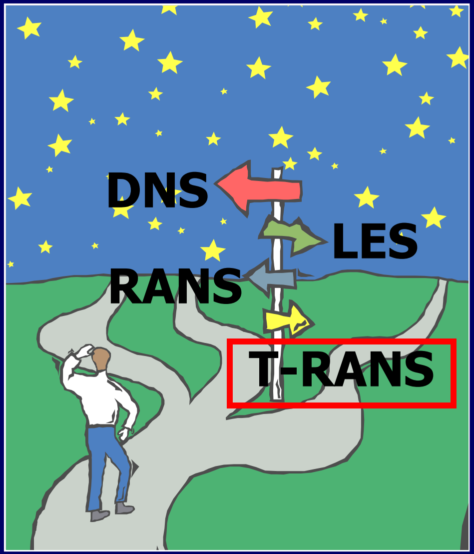
$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\right] + \frac{1}{\rho}\sum F_i$$

$$\frac{\partial B_i}{\partial t} + U_j \frac{\partial B_i}{\partial x_j} = \frac{1}{\mu_0 \sigma} \frac{\partial^2 B_i}{\partial x_j^2} + B_j \frac{\partial U_i}{\partial x_j}$$

+ divergence free conditions:

$$\partial U_i / \partial x_i = 0 \qquad \partial B_i / \partial x_i = 0$$

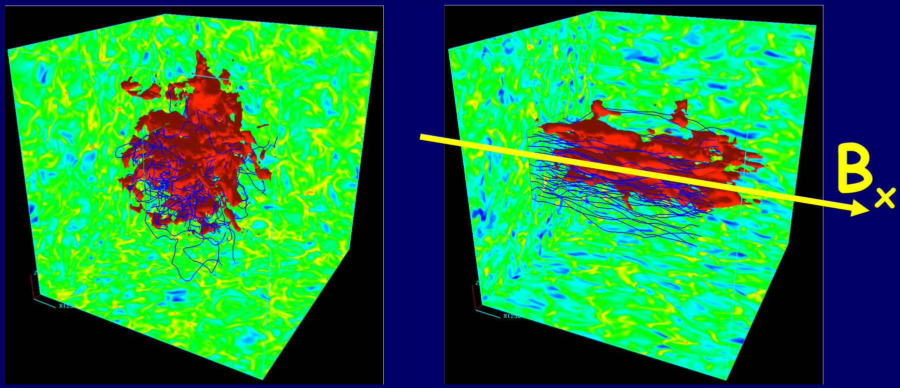
Modelling/Simulation Approach →
Hybrid T-RANS (N-S) / DNS (Maxwell)



Advanced subscale/subgrid turbulence modelling

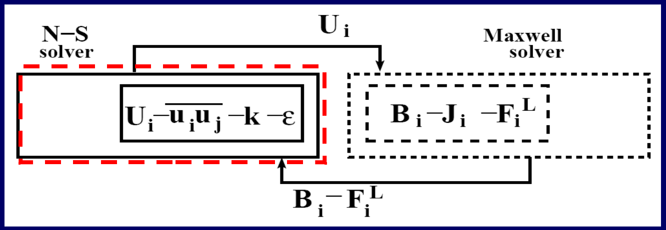
- high Re, Re_m, Ha
- Body force: strong anisotropy of turbulence
- Wall effects: viscous + blockage, low-Re
- MHD turbulence

$$\langle u_i u_j \rangle$$



$$F_i^L \longrightarrow \langle U_i \rangle \qquad f_i^L \longrightarrow u_i$$

Modelling/Simulation Approach →
Hybrid T-RANS (N-S) / DNS (Maxwell)



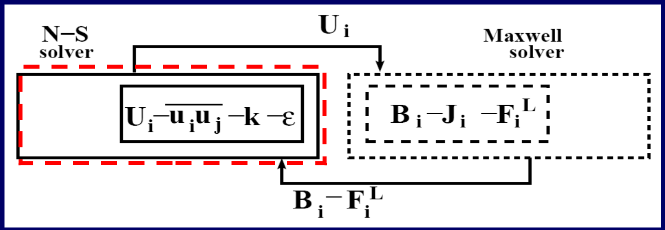
(1) Source/sink terms (production/destruction)

$$S_{ij}^{M} = \frac{\sigma}{\rho}\left(\boxed{\varepsilon_{imn} B_n \overline{e_m u_j} + \varepsilon_{jmn} B_n \overline{e_m u_i}} + B_i B_n \overline{u_j u_n} + B_j B_n \overline{u_i u_n} - 2 B_n B_n \overline{u_i u_j} \right)$$

(2) Redistributive mechanism

$$\frac{\partial^2 p}{\partial x_l^2} = -\frac{\partial^2}{\partial x_l \partial x_m}\left(\rho u_l u_m - \rho \overline{u_l u_m} \right) - 2\rho \frac{\partial U_l}{\partial x_m}\frac{\partial u_m}{\partial x_l} + \boxed{\rho \frac{\partial f_i}{\partial x_i}}$$

Modelling/Simulation Approach →
Hybrid T-RANS (N-S) / DNS (Maxwell)



(3) T-RANS subscale Second Moment Closure

$$\frac{\partial \overline{u_i u_j}}{\partial t} + U_l \frac{\partial \overline{u_i u_j}}{\partial x_l} = \frac{\partial}{\partial x_l}\left[\left(\nu \delta_{lm} + C_s \frac{k}{\varepsilon}\overline{u_l u_m}\right)\frac{\partial \overline{u_i u_j}}{\partial x_m}\right] + P_{ij} + \Phi^S_{ij} + \Phi^R_{ij} + \boxed{\Phi^M_{ij}} - \varepsilon_{ij} + \boxed{S^M_{ij}} \qquad (7)$$

Speziale, Sarkar, Gatski (1991)
+
Kenjeres and Hanjalic (2001,2004,2005)

$$\boxed{S^M_{ij} = S^{M1}_{ij} + S^{M2}_{ij}}$$

$$S^{M1}_{ij} = -\frac{\sigma}{\rho}\left(\epsilon_{ilm} B_m \boxed{\overline{u_j \frac{\partial \varphi}{\partial x_l}}} + \epsilon_{jlm} B_m \boxed{\overline{u_i \frac{\partial \varphi}{\partial x_l}}}\right)$$

$$S^{M2}_{ij} = \frac{\sigma}{\rho}\left(B_i B_l \overline{u_j u_l} + B_j B_l \overline{u_i u_l} - 2B_l^2 \overline{u_i u_j}\right)$$

$$\boxed{\overline{u_i \frac{\partial \varphi}{\partial x_j}} = C_\lambda \epsilon_{jlm} B_m \overline{u_i u_l}}$$

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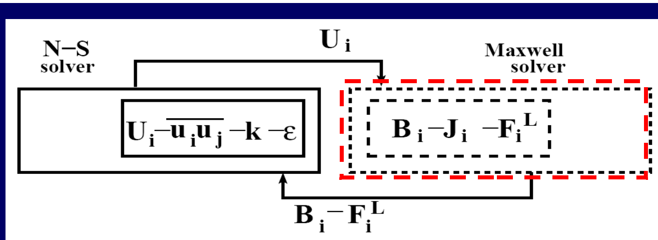
Modelling/Simulation Approach →
Hybrid T-RANS (N-S) / DNS (Maxwell)



(4) DNS for magnetic induction equations

Re_m=10-30

Pr_m=6.5x10^{-6}

$$\eta_U = \left(\nu^3/\varepsilon\right)^{1/4}$$

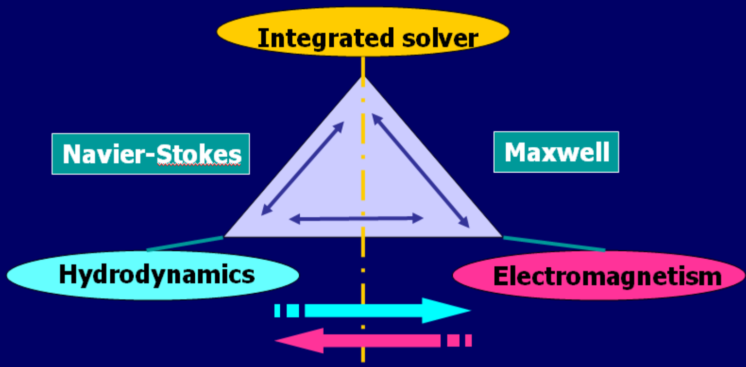
$$\eta_B = \left(\lambda^3/\varepsilon\right)^{1/4}$$

$$\rightarrow \eta_U / \eta_B = \mathrm{Pr}_m^{3/4}$$

-Magnetic diffusive length scales >> velocity viscous scales

-Experimentally observed frequencies of magnetic field ~ 1 Hz

Numerical Solver and Computational Mesh



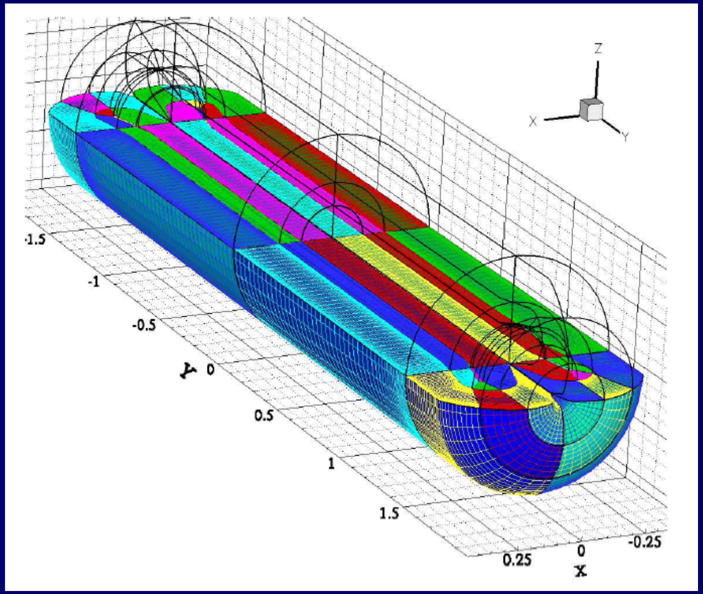
-Finite volume second-order for the non-orthogonal multi-domain/multi-block

-TVD (UMIST limiter) for convective terms

-CDS for diffusive terms

-fully implicit three-time steps integration

-MPI (32-128 CPUs) SGI-Altix



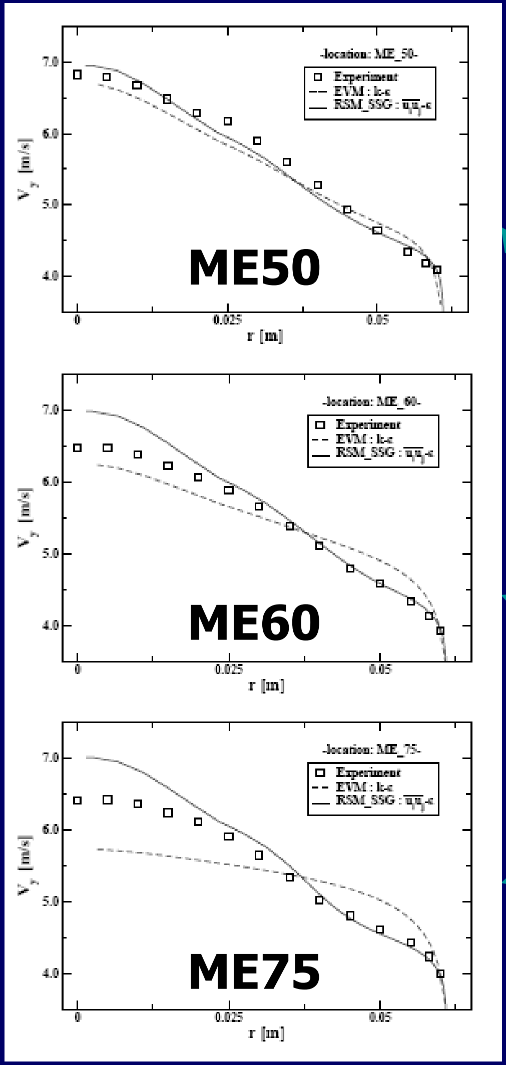
-Numerical mesh: 90 multi-blocks with ~4×10^6 CVs

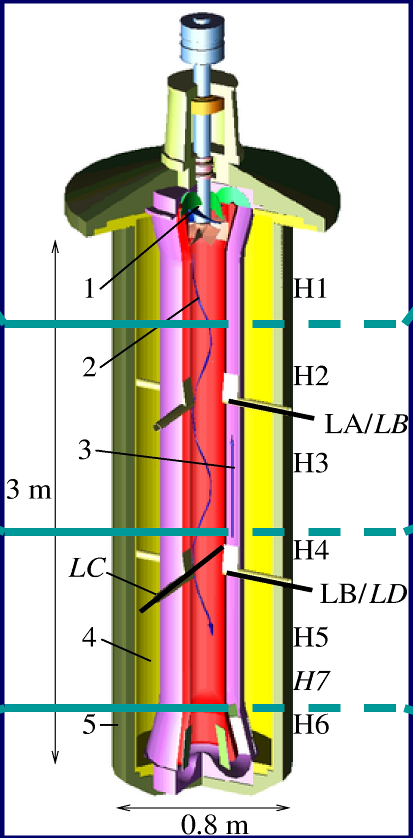
-Wall-functions for velocity and turbulence variables $45 < (x^+, z^+) < 100$

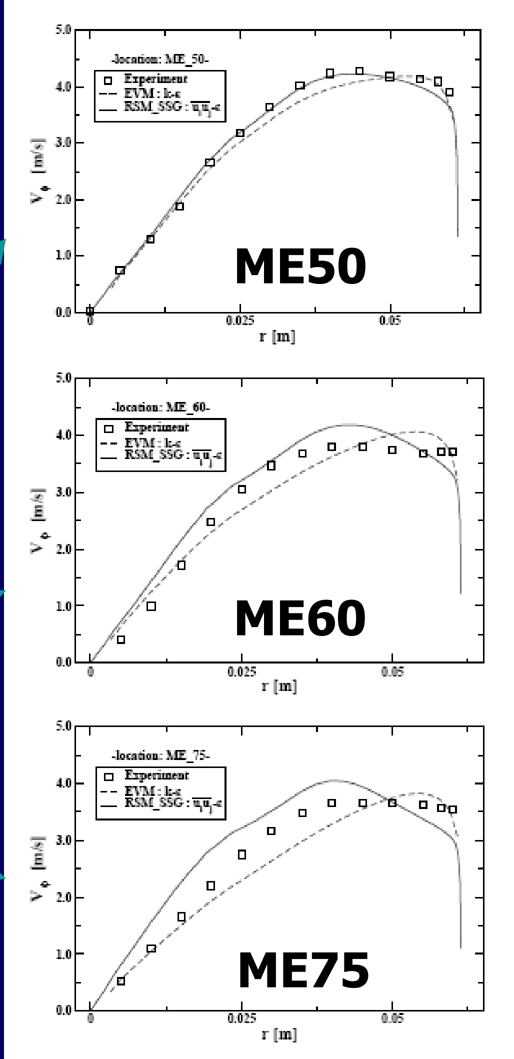
-Vertical magnetic field condition in order to allow natural escape of self-generated magnetic field

-Time step: $\Delta t \sim 1/100$ of the experimentally observed periods

-1:2 water model-







-axial velocity-

-tangential velocity-

-1:2 scale-down water model of the Riga dynamo setup: comparison with LDA measurements in the inner cylinder, Christen *et al.* (2002)

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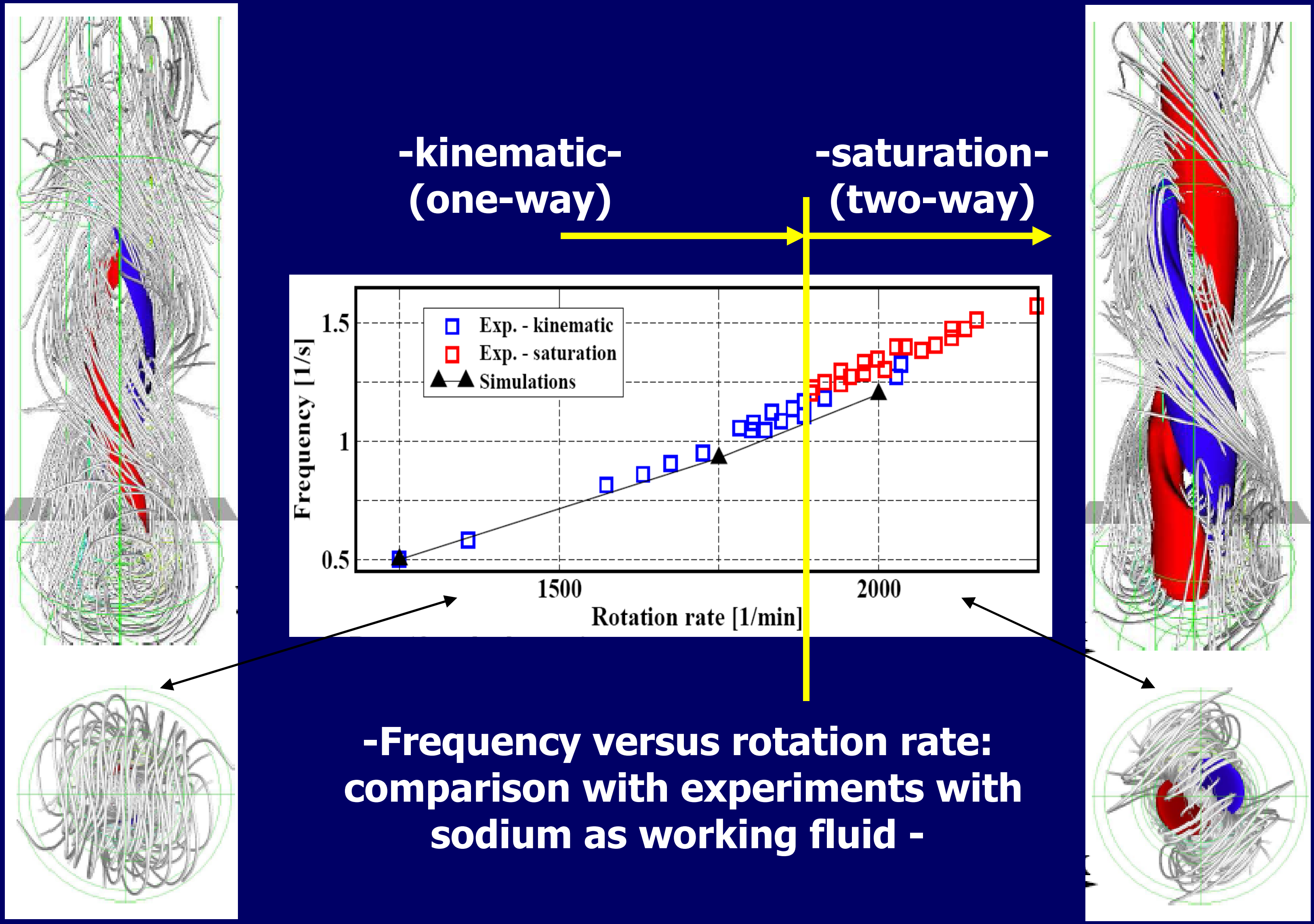
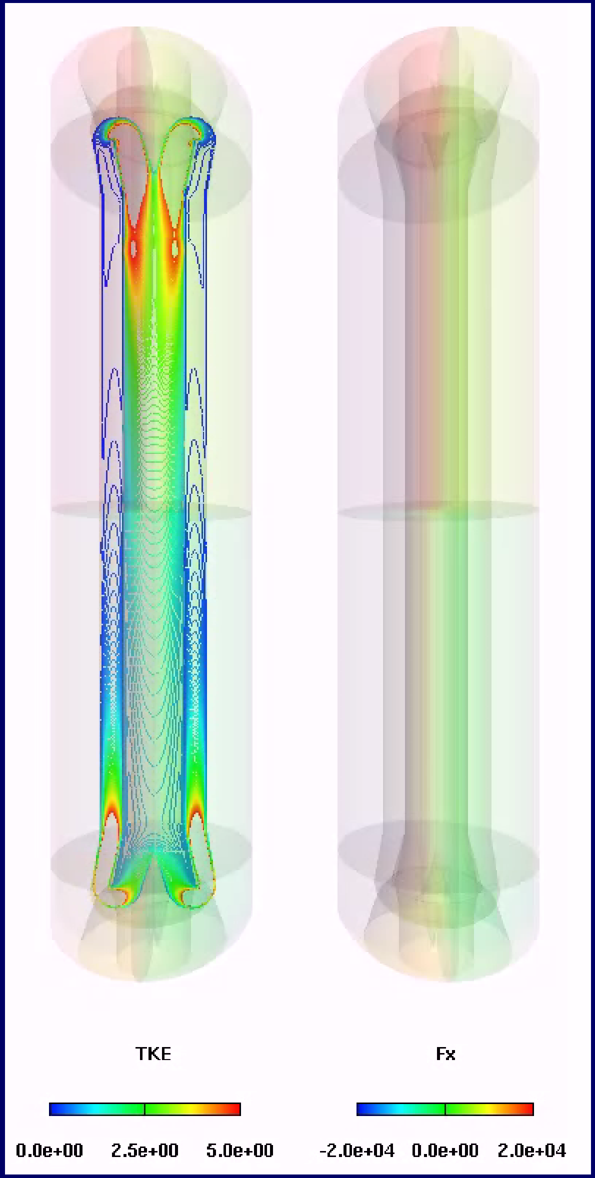
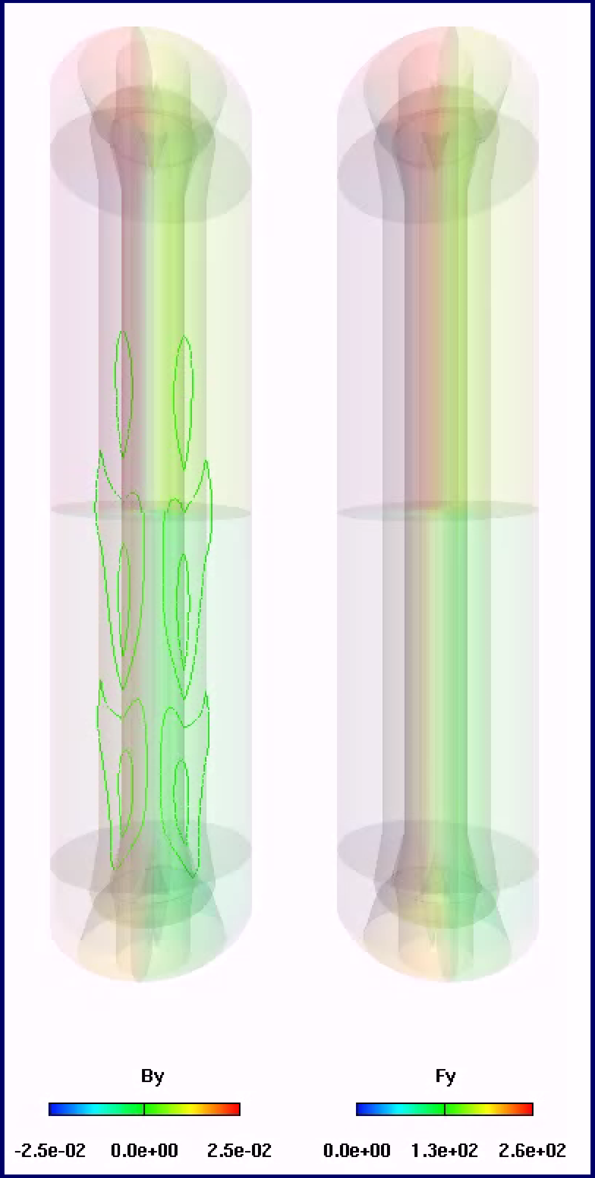


-Frequency versus rotation rate: comparison with experiments with sodium as working fluid -

-Full scale Riga dynamo setup with sodium: comparison of frequencies of generated magnetic field (experiments Gailitis *et al.* , 1999-2005)





Time evolutions in the central vertical plane: TKE-Fx, By-Fy (axial) ~ 6.5 sec of real time.

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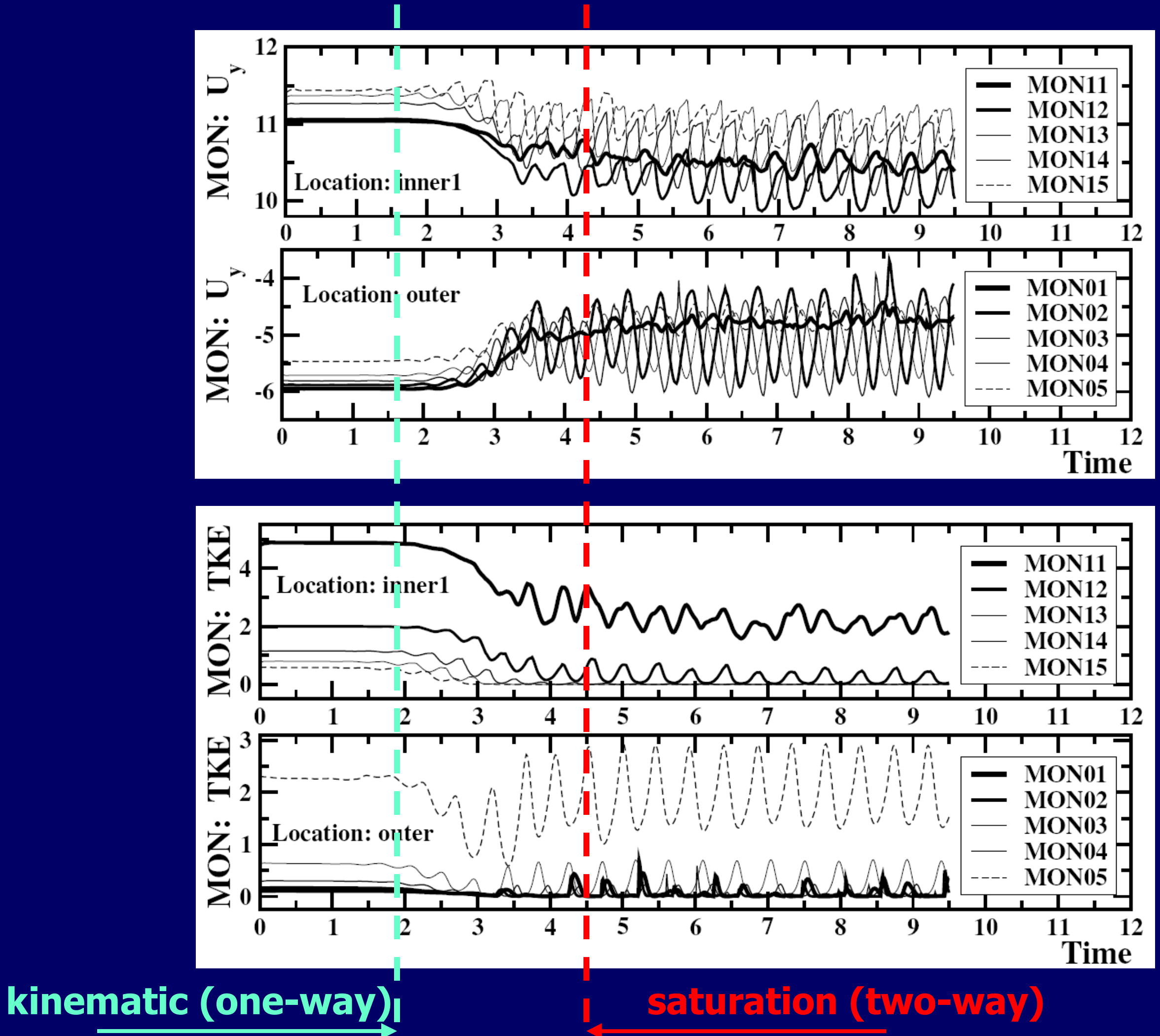
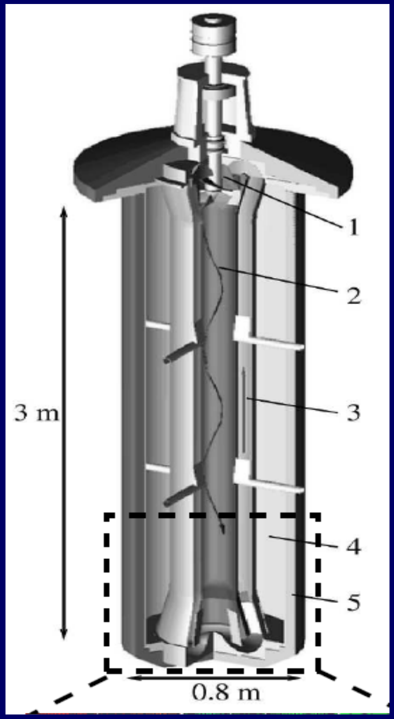
Time Evolutions of Axial Velocity and TKE



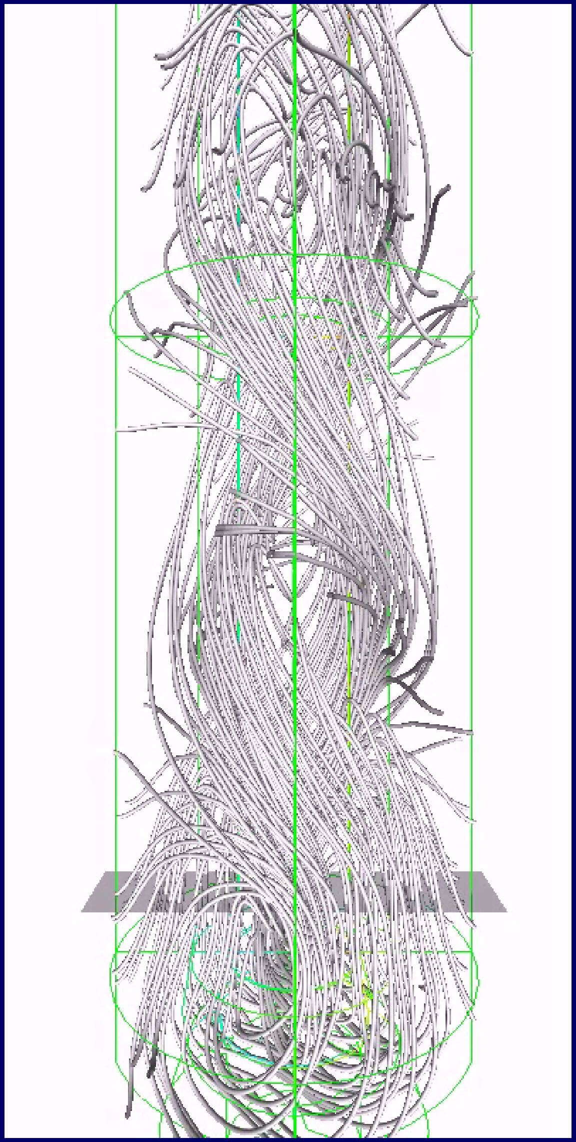
U_y → suppressed

TKE → suppressed

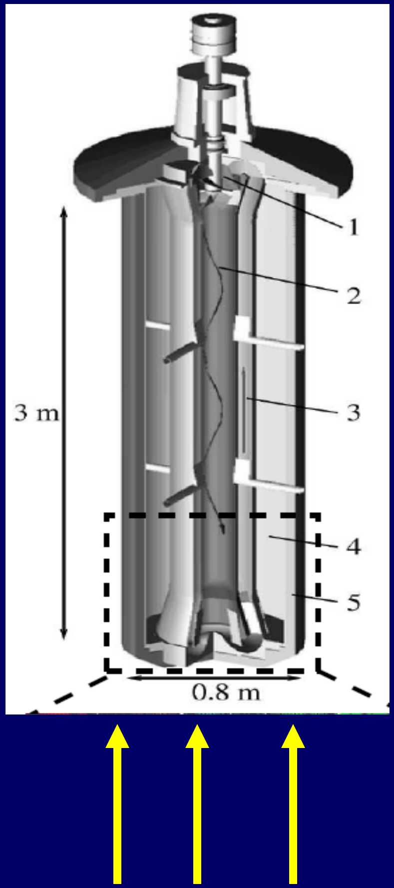
TKE → enhanced



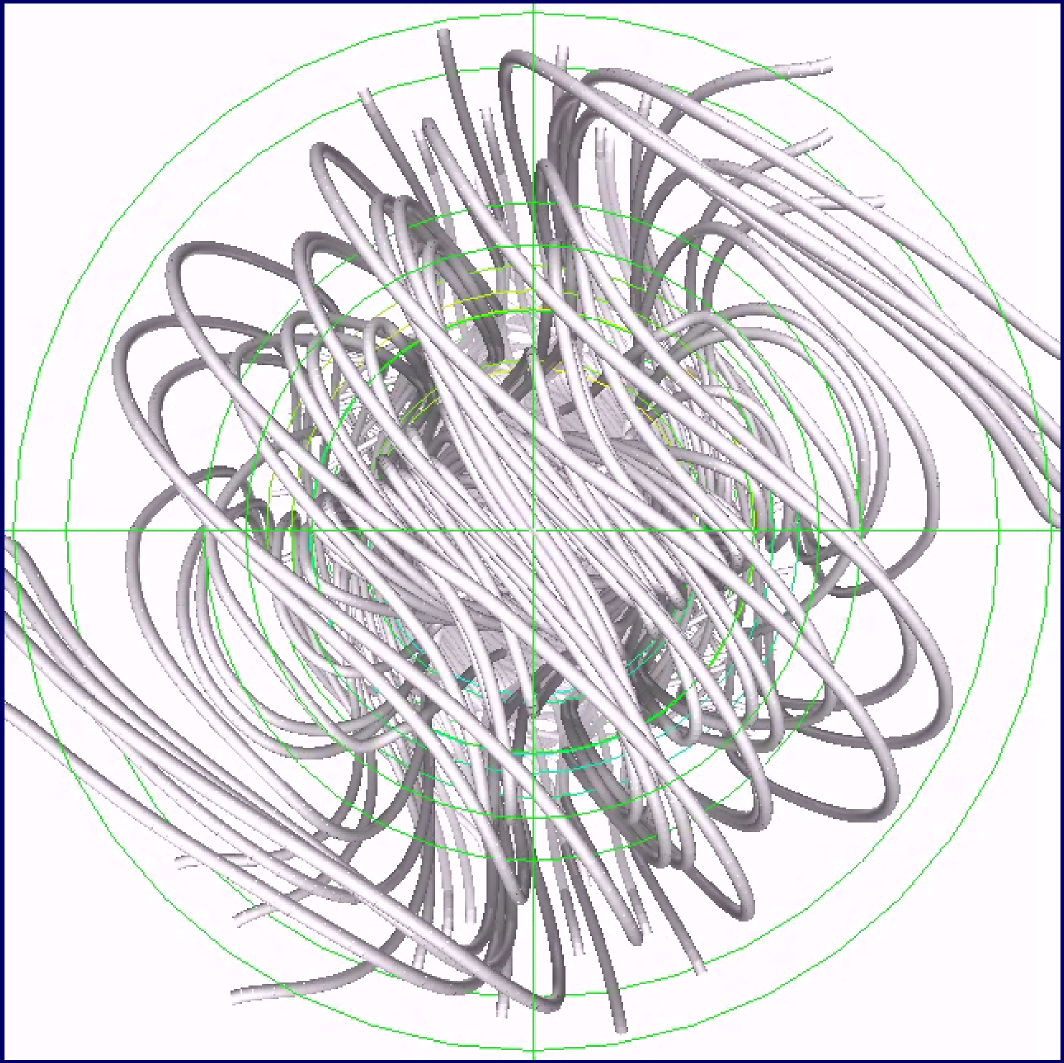
-view from side-



-Time evolution of the axial magnetic field component isosurfaces (B_y=0.02 – red., -0.02-blue) with magnetic flux lines (grey tubes) → view from side.



-view from below-



-Time evolution of the axial magnetic field component isosurfaces (B_y=0.02 – red., -0.02-blue) with magnetic flux lines (grey tubes) → view from below.

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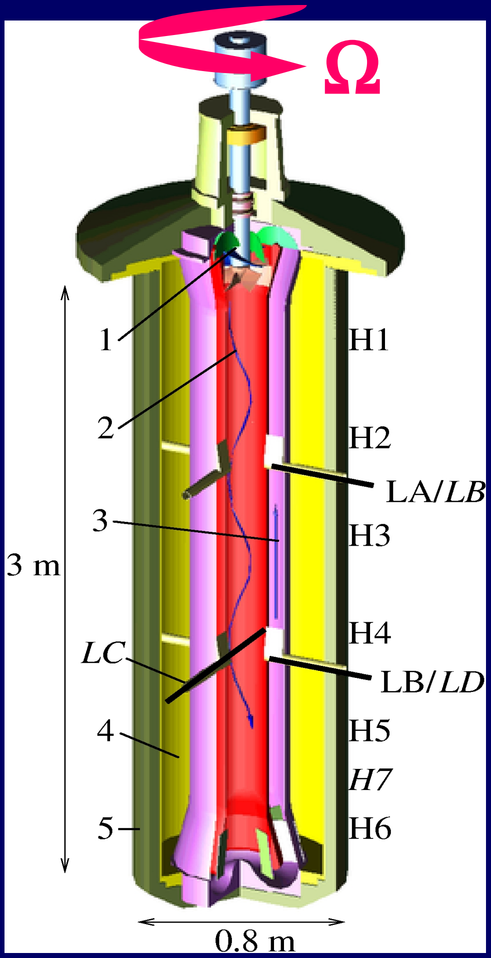
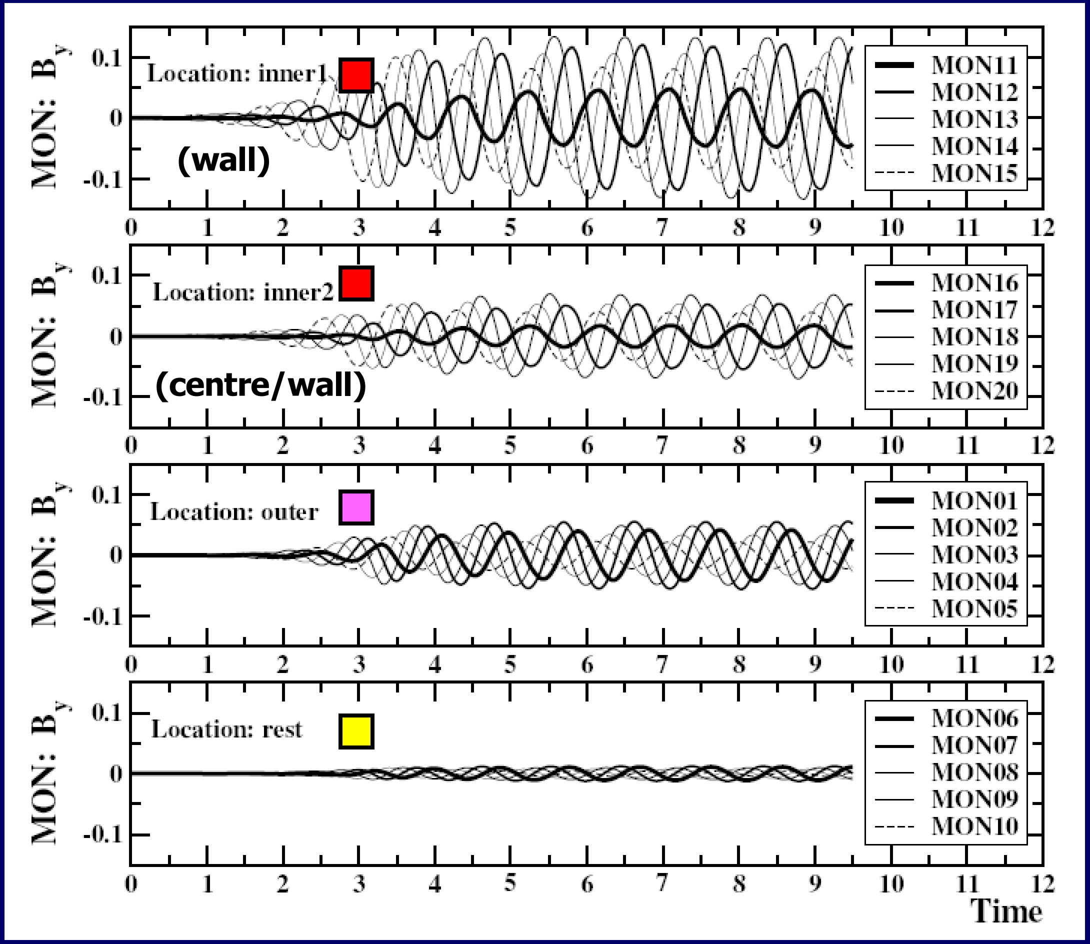
Time Evolutions of Self-Generated Magnetic Fields





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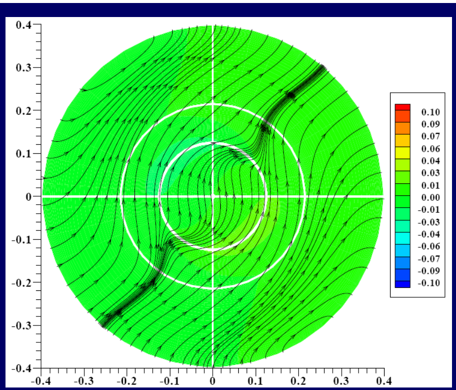
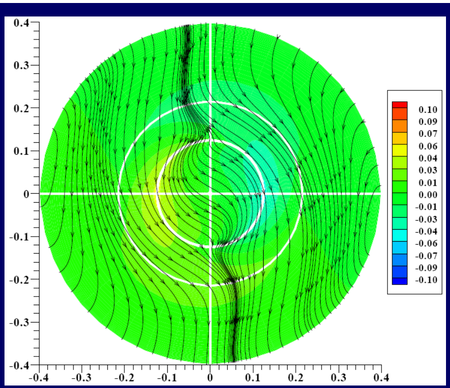
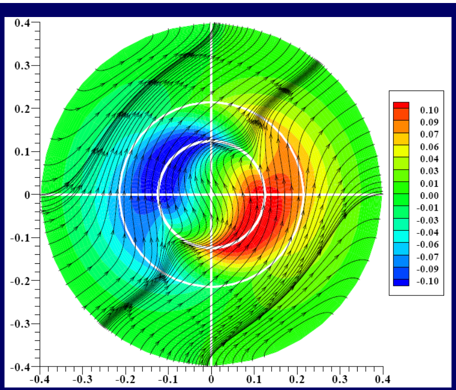
Comparisons with Experiments:

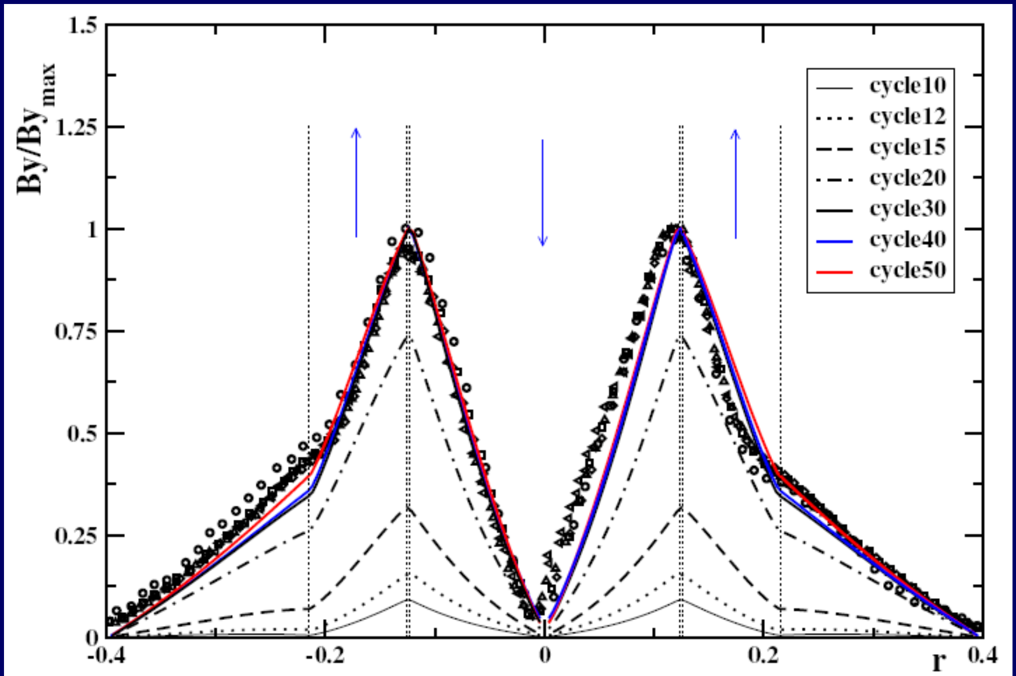


cycle15



cycle45





- Axial magnetic field-

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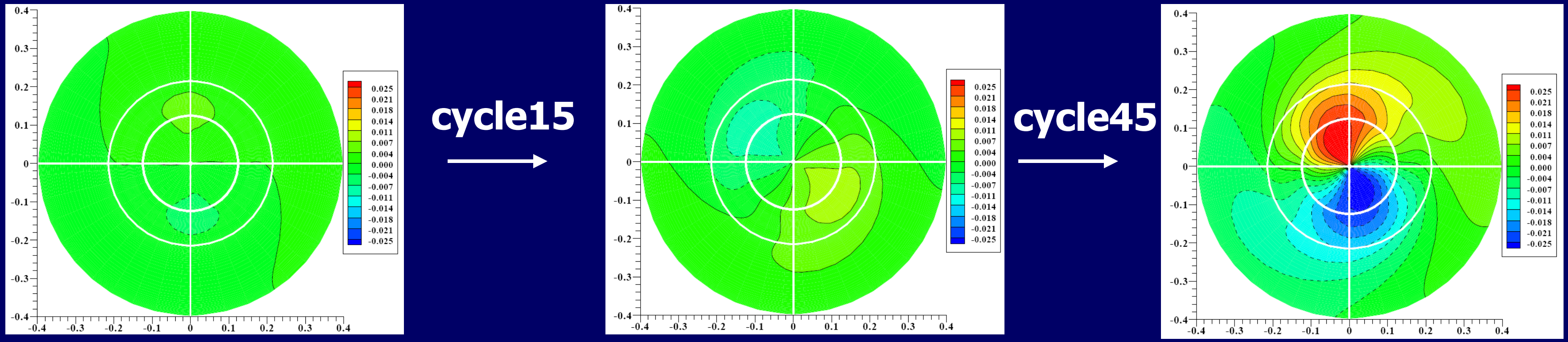
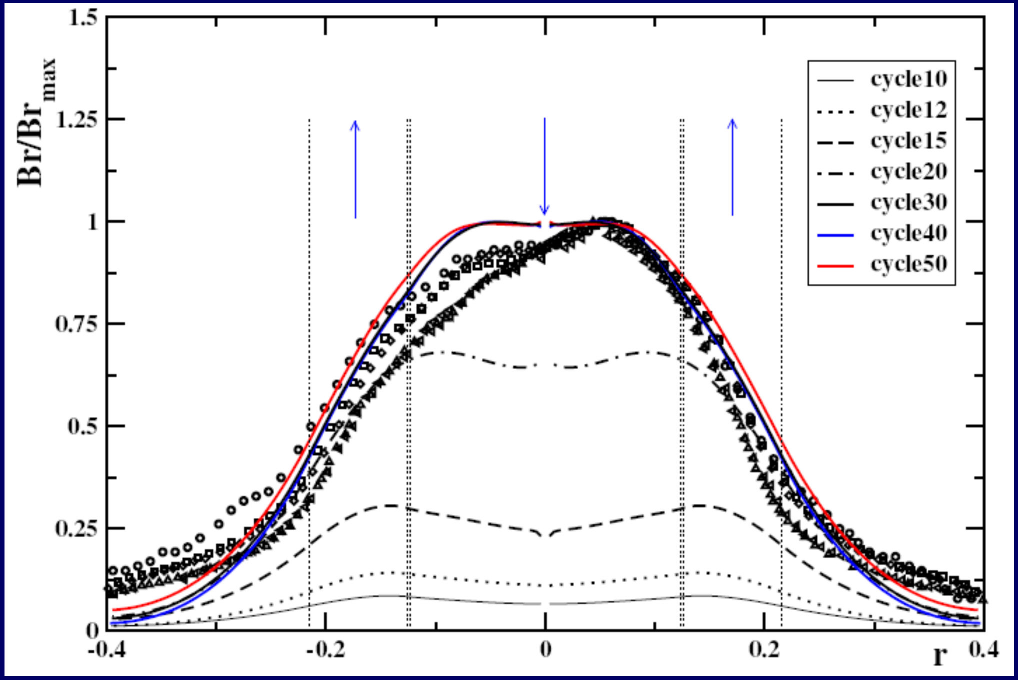
Comparisons with Experiments:





- Radial magnetic field-

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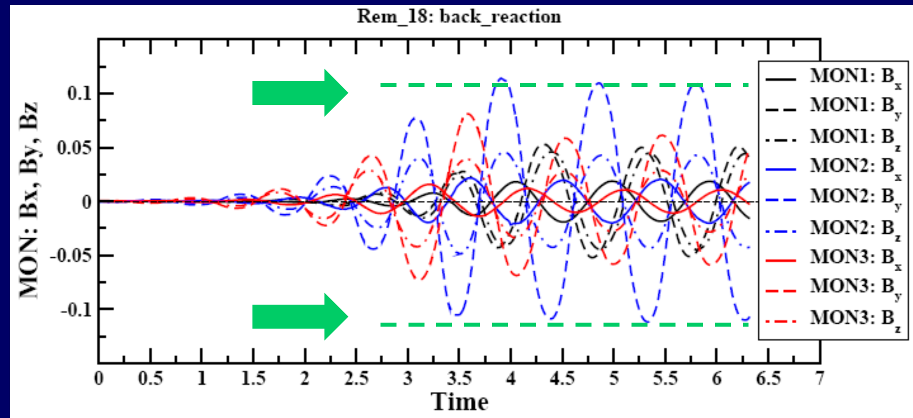
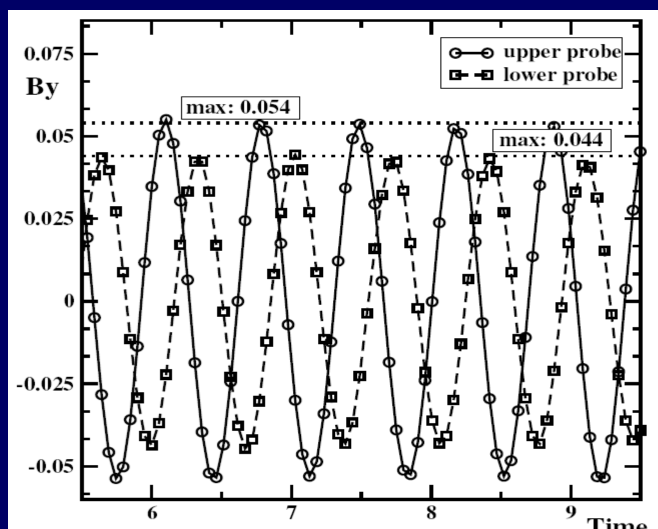
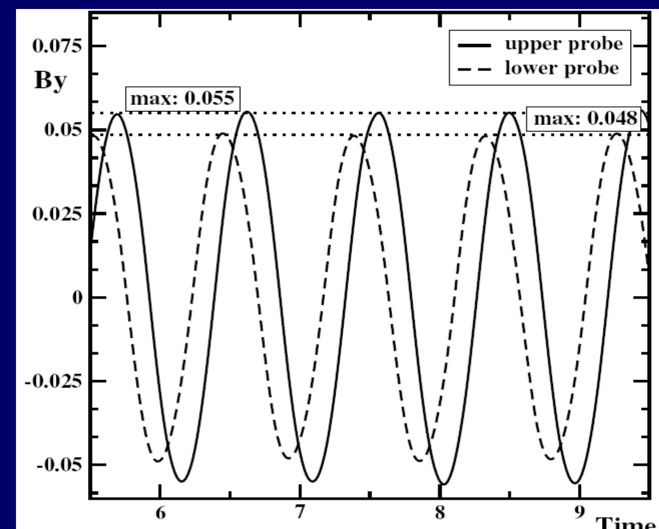
Comparisons with Experiments:

$$U_i \xrightarrow{Convection} B_i$$

$$B_i \xrightarrow{LorentzForce} U_i$$







-experiment- **-simulation-**

Conclusions:

- It is demonstrated that two-way coupled turbulent magnetic dynamo in complex geometry was successfully numerically simulated

- Application of hybrid T-RANS/DNS approach made it possible to mimic flow and magnetic regimes up to now inaccessible to other simulation techniques (DNS, LES)

- It is proved that the action of the hydro-magnetic dynamo in turbulent regime can naturally produce and self-sustain a magnetic field without any external excitation or artificial inputs

Towards More Efficient Drug Delivery: Blood Flow in Stenotic Arteries Subjected to a Strong Non-Uniform Magnetic Field

Motivation:

- Ongoing challenge of chemotherapy: to provide specific delivery of chemotherapeutic agents to their desired targets with a minimum of systemic side effects

- Locoregional Cancer Treatment with Magnetic Drug Targeting (MDT)

- Mathematical modelling and numerical simulations as a tool for further advancements of Magnetic Drug Targeting: Fluid Mechanics / Electromagnetism

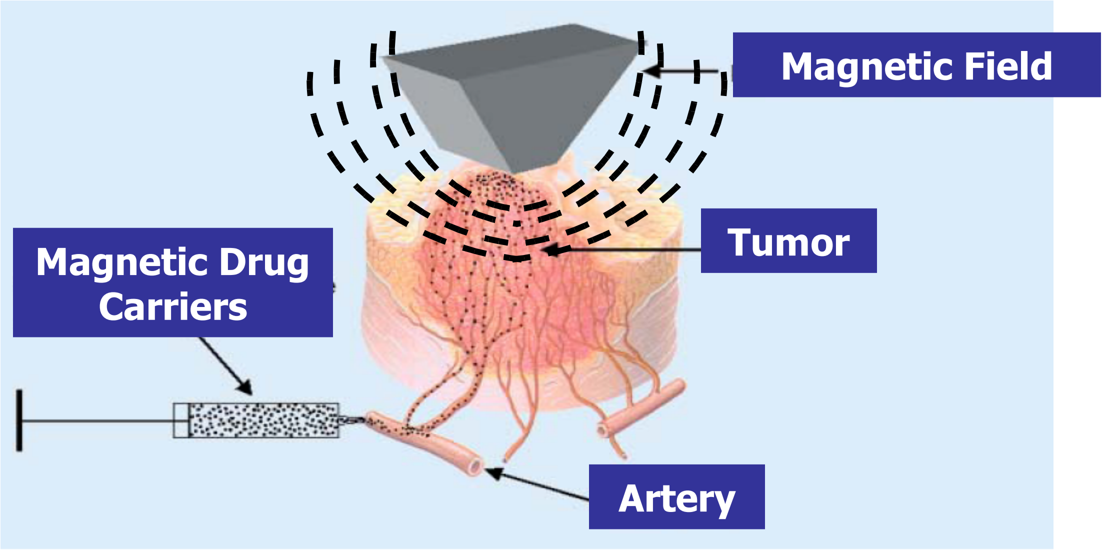
Goal:

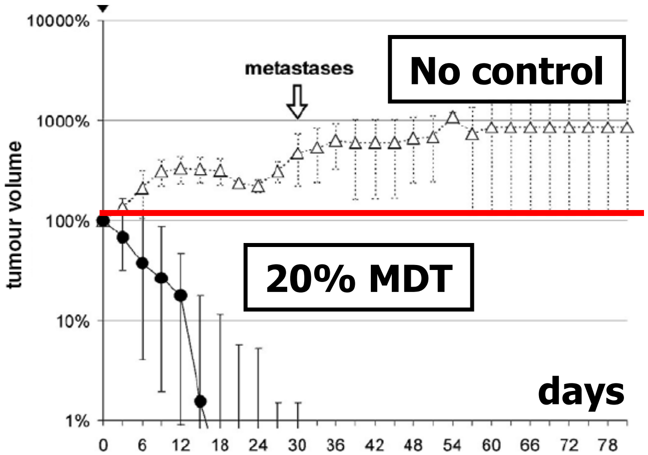
- To provide insights into fundamental physics of blood flow subjected to strong external magnetic fields

- *A priori* personalised parametric studies mimicking individual patient conditions

- Tailoring optimised magnetic fields (strength, gradients, penetrative capabilities) for bio-medical applications

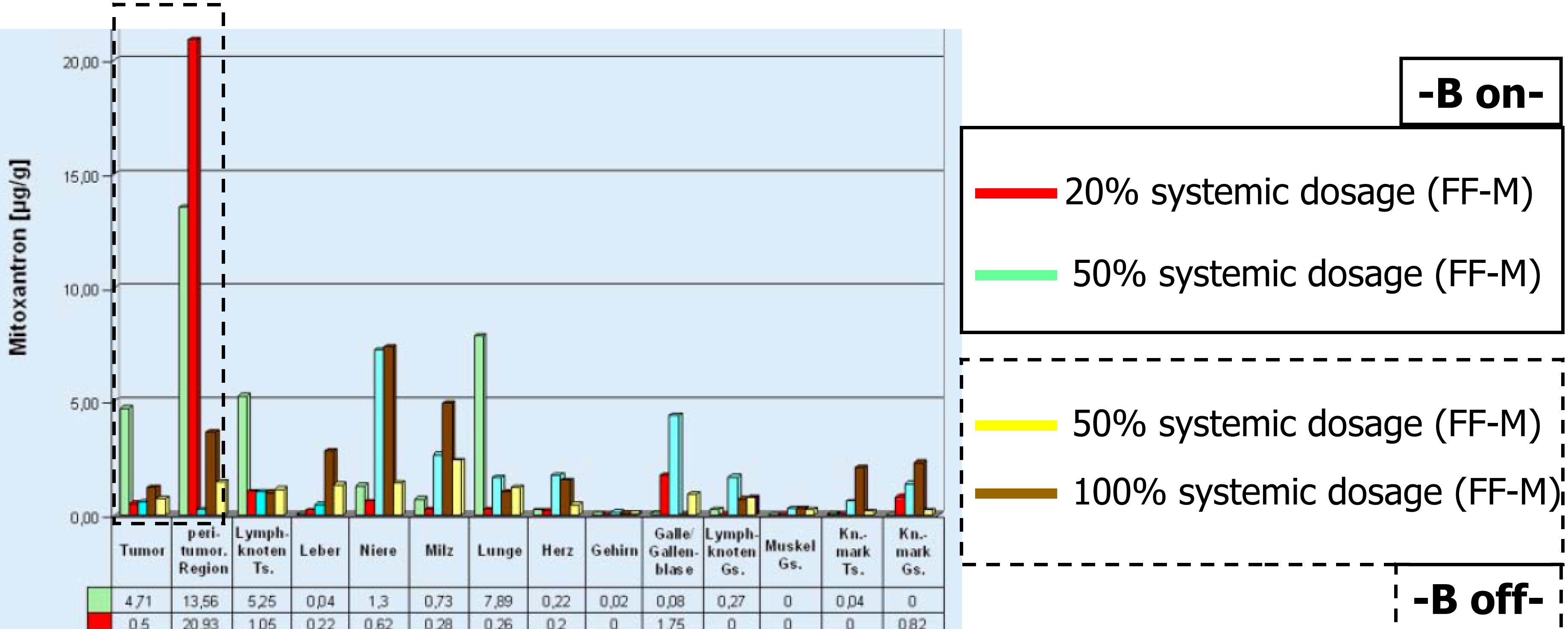
-Principles of local chemotherapy with Magnetic Drug Targeting-
Alexiou et al. (2003,2005,2006)





Rabbits with limb tumor 40 days after treatment:
A) 20% of systemic dose with MDT
B) 75% regular systemic dose

-Mitoxantron concentrations 60 min after application: B=0.6 [T]



	Tumor	peri-tumor. Region	Lymph-knoten Ts.	Leber	Niere	Milz	Lunge	Herz	Gehirn	Galle/ Gallen-blase	Lymph-knoten Gs.	Muskel Gs.	Kn.-mark Ts.	Kn.-mark Gs.
	4,71	13,56	5,25	0,04	1,3	0,73	7,89	0,22	0,02	0,08	0,27	0	0,04	0
	0,5	20,93	1,05	0,22	0,62	0,28	0,26	0,2	0	1,75	0	0	0	0,82
	0,58	0,25	1,03	0,47	7,29	2,65	1,66	1,75	0,12	4,38	1,69	0,32	0,62	1,39
	1,23	3,65	0,99	2,83	7,42	4,91	1	1,55	0,07	0	0,73	0,3	2,1	2,3
	0,75	1,45	1,16	1,34	1,42	2,41	1,24	0,46	0,07	0,91	0,8	0,24	0,18	0,22

-Experimental animal studies-
Alexiou et al. (2005)
HNO Vol.53, pp.618-622

Conclusions:
20 – 50 % smaller drug dosage
26 times higher local concentrations

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Mathematical Model:

Navier-Stokes/Maxwell's Equations

$$\nabla \cdot \mathbf{V} = 0, \quad \nabla \cdot \mathbf{B} = 0 \qquad (1)$$

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla)\, \mathbf{V} = \nu \nabla^2 \mathbf{V} + \frac{1}{\rho} \left[-\nabla P + \underbrace{\mathbf{J} \times \mathbf{B}}_{\mathbf{F}^{\mathrm{L}}} + \underbrace{\mu_0 (\mathbf{M} \cdot \nabla)\, \mathbf{H}}_{\mathbf{F}^{\mathrm{M}}} \right] \qquad (2)$$

$$\nabla \times \mathbf{H} = \mathbf{J}, \quad \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = \sigma (\mathbf{E} + \mathbf{U} \times \mathbf{B}) \qquad (3)$$

F^L – Lorentz force
(moving electroconducting fluid through imposed **B**)

F^M – Magnetization force
(magnetisation response due to non-uniform **B**)

Mathematical Model:

Plasma + Red Blood Cells + White Blood Cells + Platelets = Blood

$6\text{-}8 \times 10^{-6}$ m

$2\text{-}4 \times 10^{-6}$ m

Homogeneous fluid for blood vessels $D > 10^{-4}$ m, Pedley (1980)

Newtonian or Non-Newtonian fluid?

Shear rates > 100 s^{-1}

Pedley (1980)

Entire cardiac cycle

30% of cardiac cycle non-Newtonian

Johnston et al. (2004,2006)

Models: Carreau, Walburn-Schneck,
Power Law, Cassau, Generalised Power Law, …

Mathematical Model:

Magnetisation force modelling

Berkovsky et al. (1993), Odenbach (2002):

$$M = n \cdot m \cdot L(\xi) = n \cdot m \left(coth\ \xi - \frac{1}{\xi} \right), \quad \xi = \frac{\mu_0 m H}{\kappa T} \qquad (4)$$

Berkovsky et al. (1993), Rosensweig (2002), Tzirtzilakis (2005) (isothermal conditions):

$$M = \chi H \qquad (5)$$

F^M – Magnetization force
(present: simple, non-isothermal, new model)

Table 1: Properties of the bio-magnetic fluid (blood) used for numerical simulations.

ρ	ν	σ	χ^{oxyg}	χ^{deoxyg}
1050.	4×10^{-6}	$0.7 - 0.9$	-6.6×10^{-7}	3.5×10^{-6}

???

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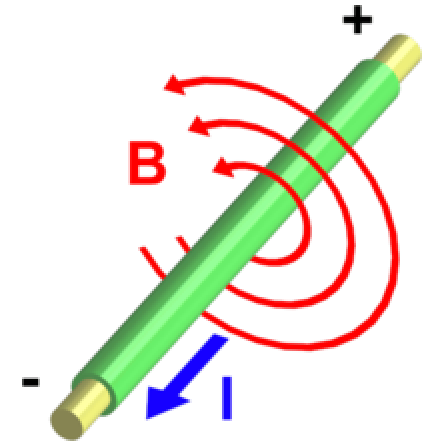
Mathematical Model:

Magnetic field distributions



Biot-Savart law:

$$B = \frac{\mu_0 I}{2\pi R} \rightarrow B_x = -\mu_0 \sum_{i=1}^{N} \frac{I_i\left(y - y_i^c\right)}{\left(x - x_i^c\right)^2 + \left(y - y_i^c\right)^2}, \quad B_y = \mu_0 \sum_{i=1}^{N} \frac{I_i\left(x - x_i^c\right)}{\left(x - x_i^c\right)^2 + \left(y - y_i^c\right)^2} \tag{6}$$

$$B(x, y, z) = \sqrt{B_x^2 + B_y^2 + B_z^2} \tag{7}$$

Lorentz force: (JxB)

Ohm's law for moving media + Kirchhoff current continuity condition

$$\mathbf{J} = \sigma\left(\mathbf{E} + \mathbf{U} \times \mathbf{B}\right)$$

(inductionless assumption)

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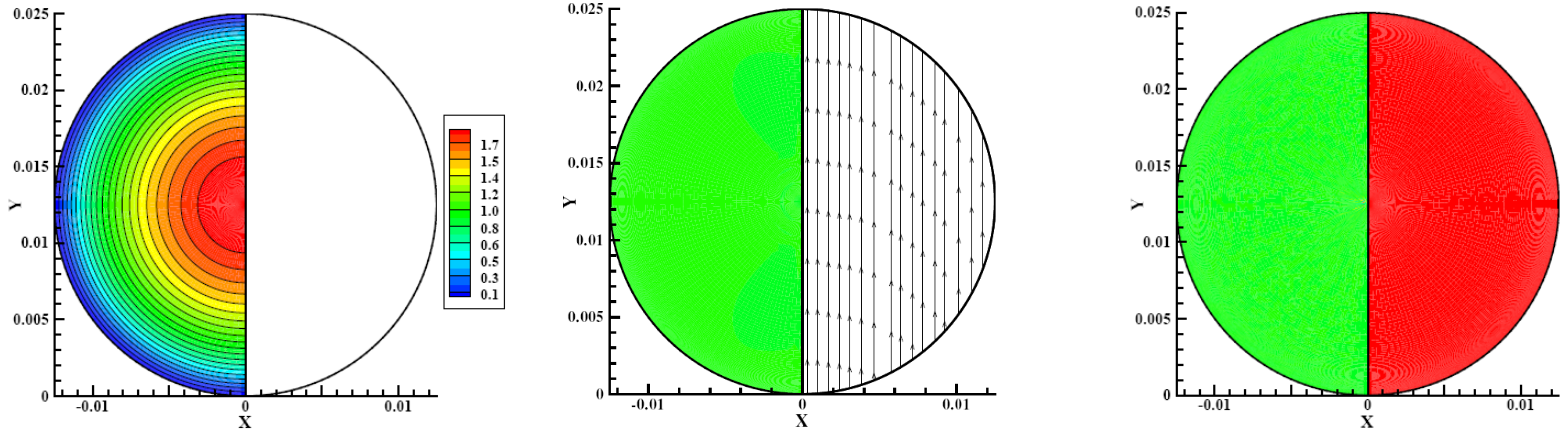
MODEL(S) VALIDATION AND APPLICATIONS:

(I) Steady blood flow in a horizontal cylinder subjected to non-uniform B

(II) Steady and pulsating blood flow in realistic stenotic arteries

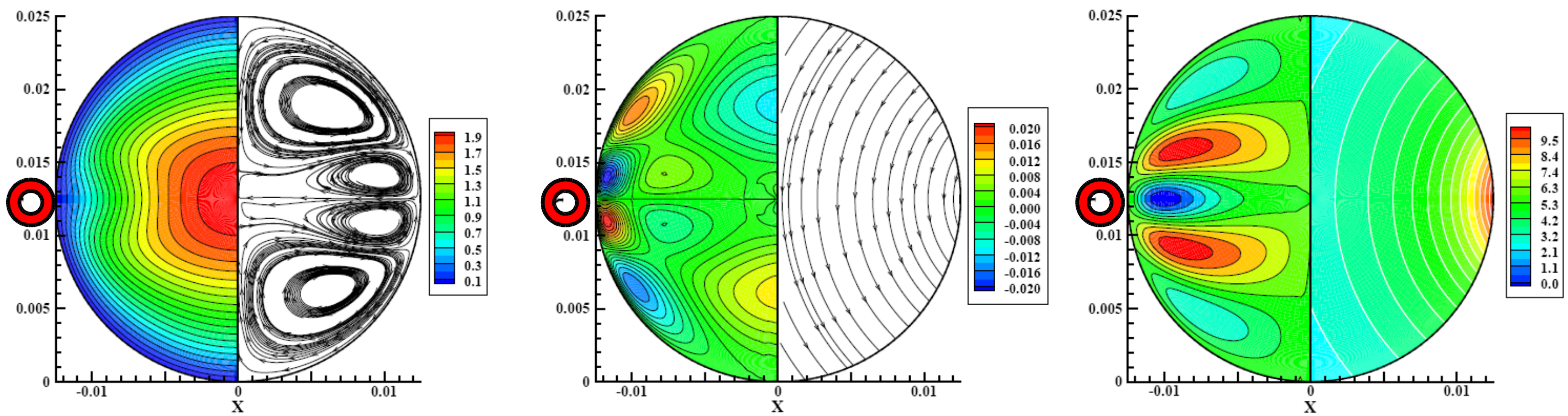
(III) Steady blood flow in stenotic arteries subjected to non-uniform B



Uniform B

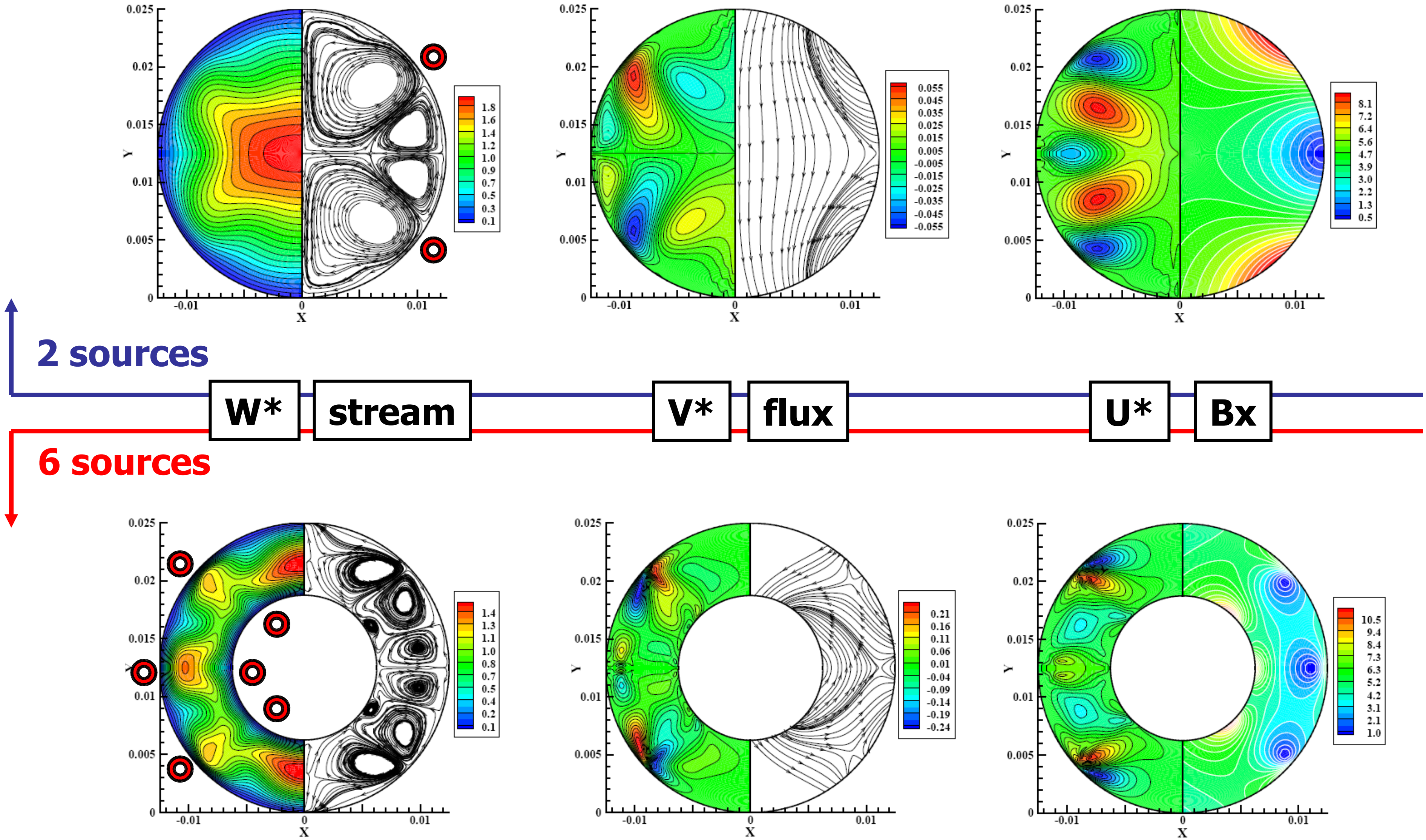
W* **stream** **V*** **flux** **U*** **Bx**

Non-uniform B



W*=W/Wmax, U*=U/Wmax
82^3 CVs + QUICK

Re~500, |B|=0 - 10 T



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$Re \sim 500$, $|B| = 0 - 10$ T

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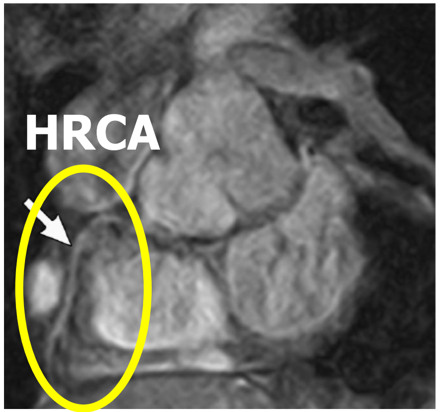
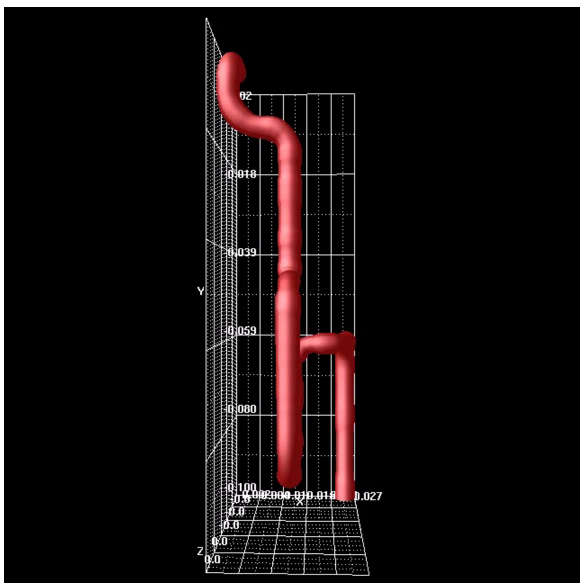
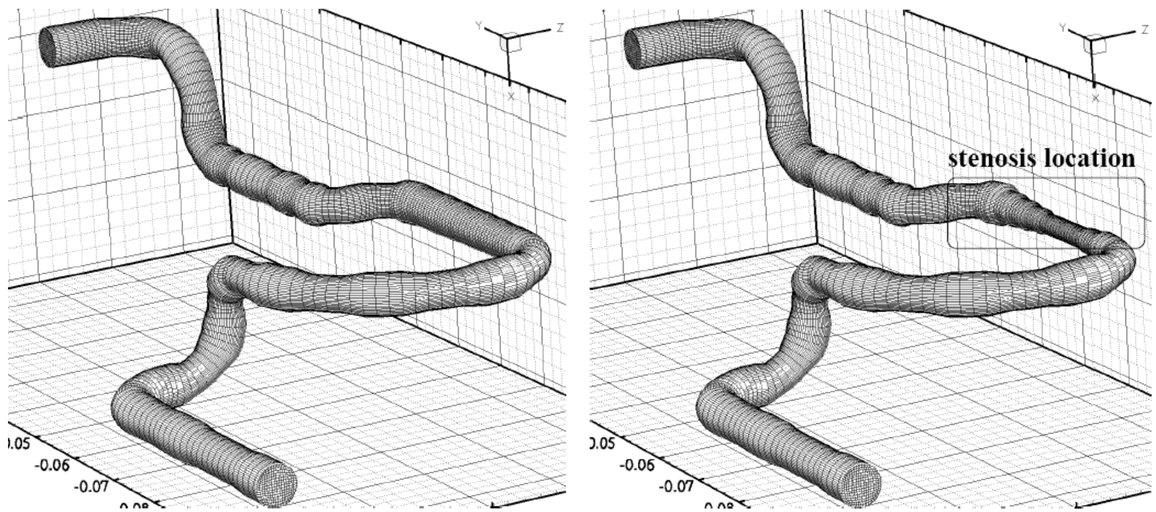
Human right coronary artery (HRCA) → X-ray angiogram to geometrical model



Johnston et al. (2004,2006)
Journal of Biomechanics 37, 39
(steady + transient, no stenosis)

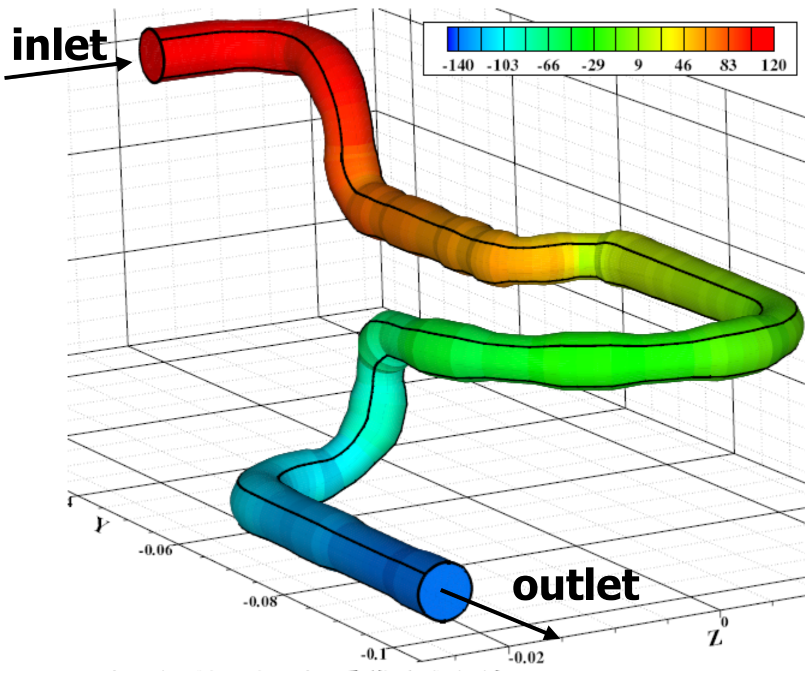




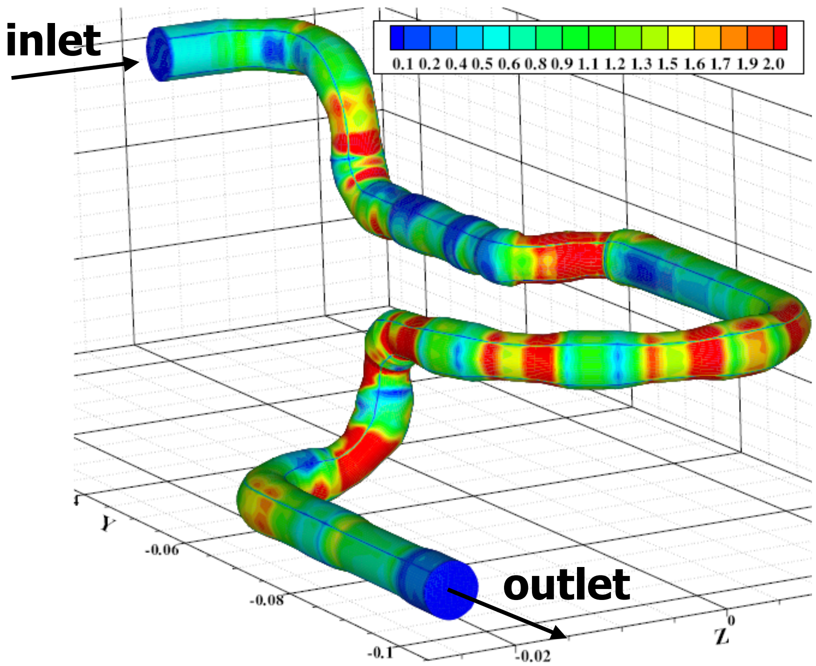
Numerical mesh: 38^2x 236 CVs, 4-8 CPUs MPI

D~5 mm, Re~500

Numerical simulations (healthy artery: 0% stenotic) – steady



-pressure along the vessel wall-



-WSS along the vessel wall-

WSS in good agreement with Johnston et al. (2004, 2006): 0 < WSS < 4 Pa

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Re~500

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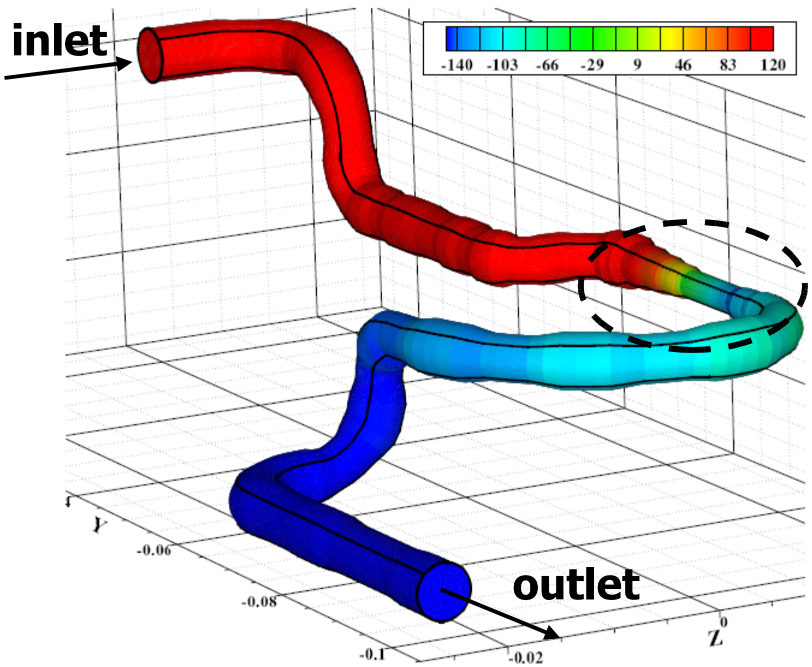
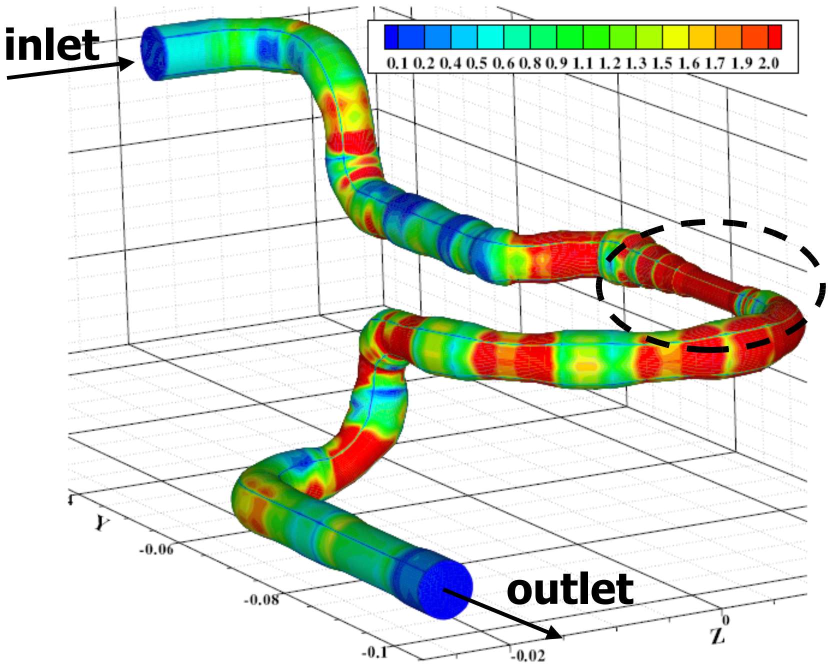
Numerical simulations (50% stenotic artery) – steady



-pressure along the vessel wall-



-WSS along the vessel wall-

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Re~500

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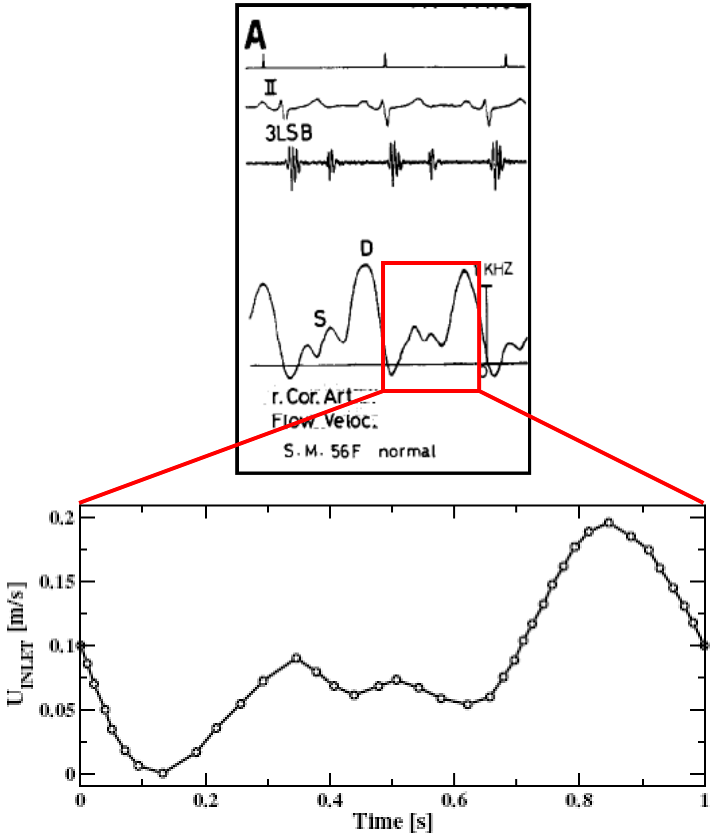
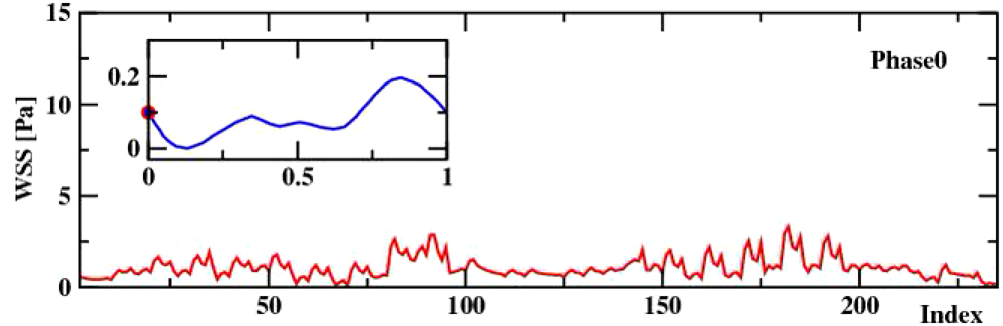
Doppler Flowmeter Catheter recordings:

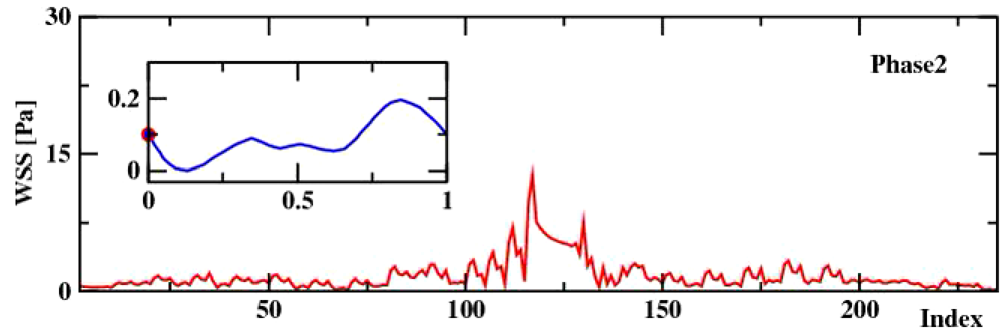


Realistic pulsating cycle:
56 years female
Matsuo et al. (1988)

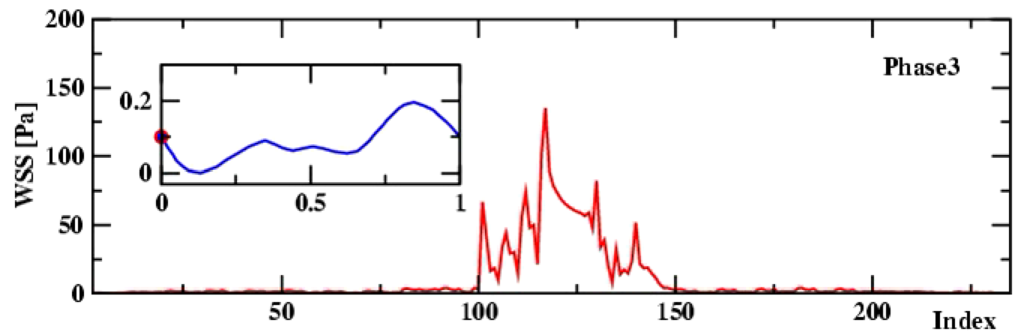
The Americal Journal of Cardiology 62



-stenosis growth: 0%



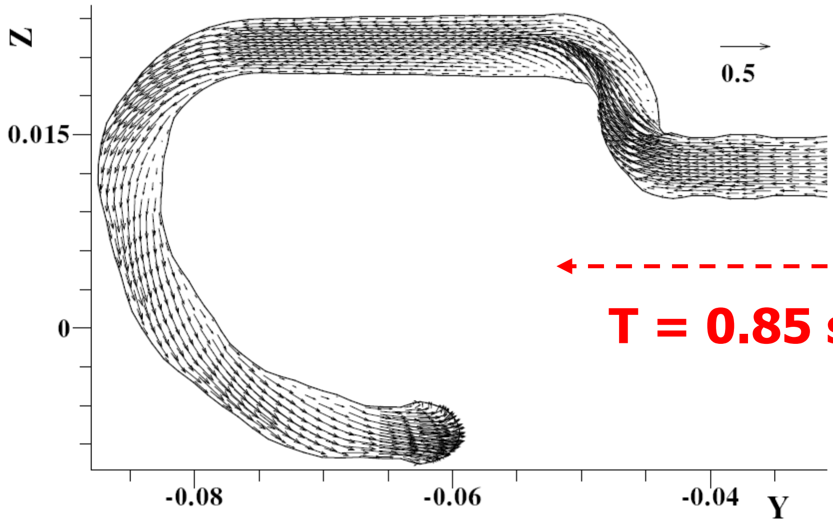
-stenosis growth: 50%



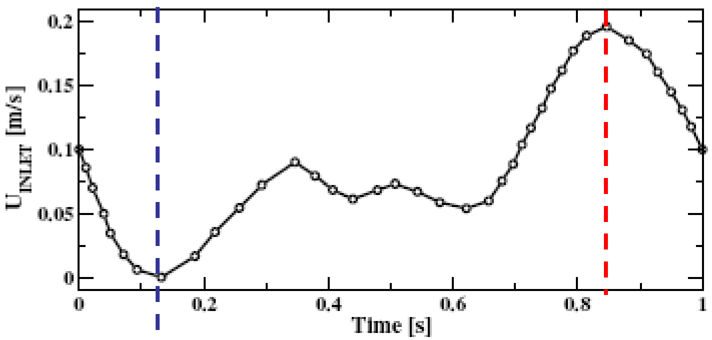
-stenosis growth: 75%

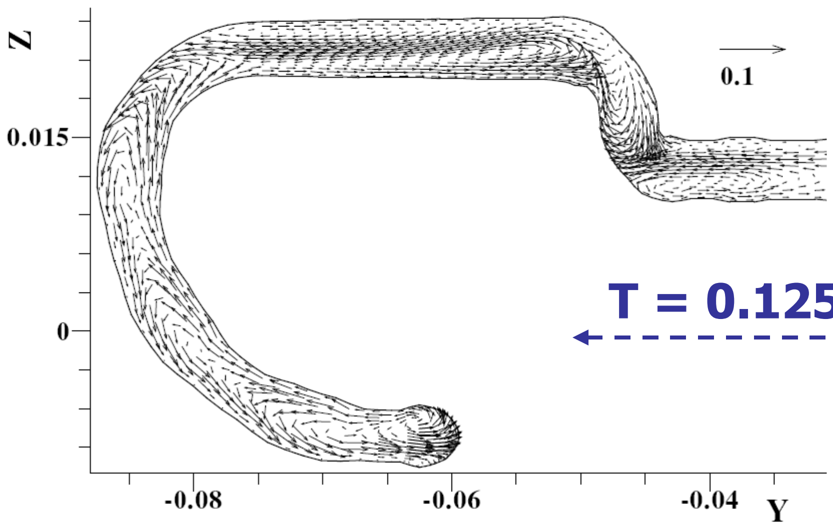
-WSS circumferentially averaged along the arc-length-

Numerical simulations (healthy artery: 0% stenotic) – pulsating



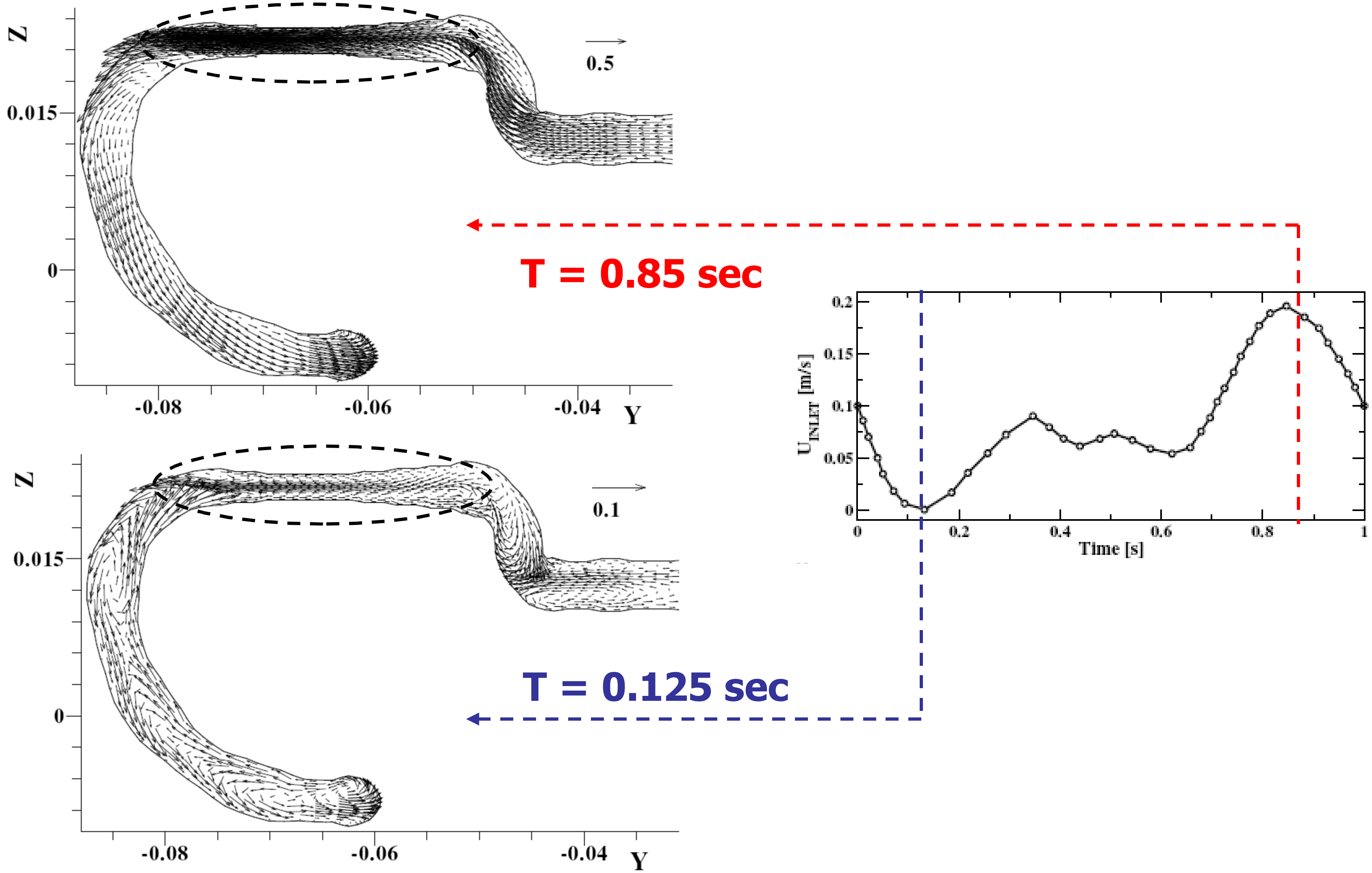
T = 0.85 sec





T = 0.125 sec

Numerical simulations (50% stenotic artery:) – pulsating



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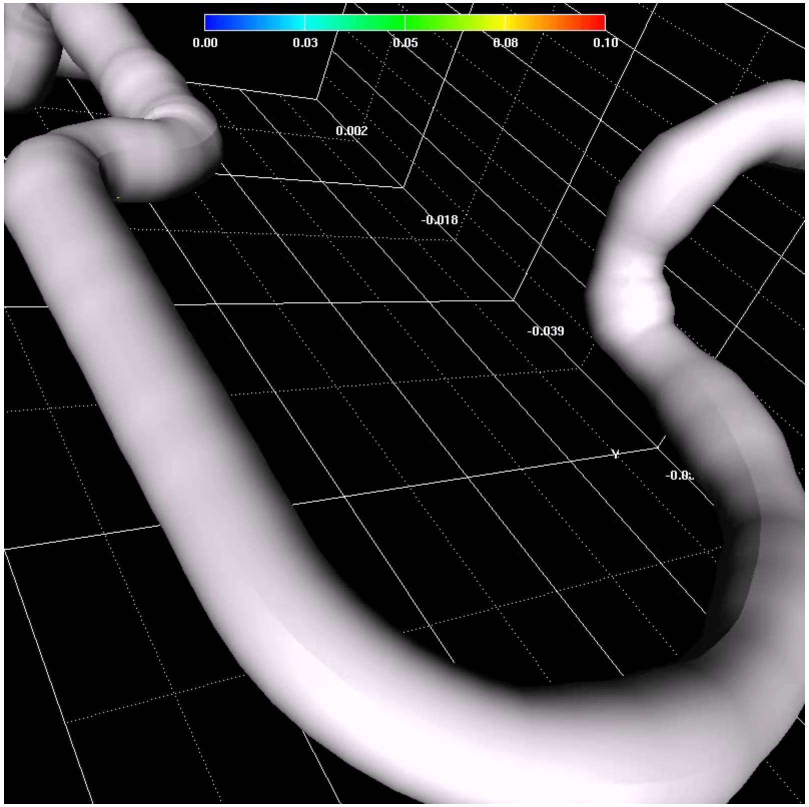
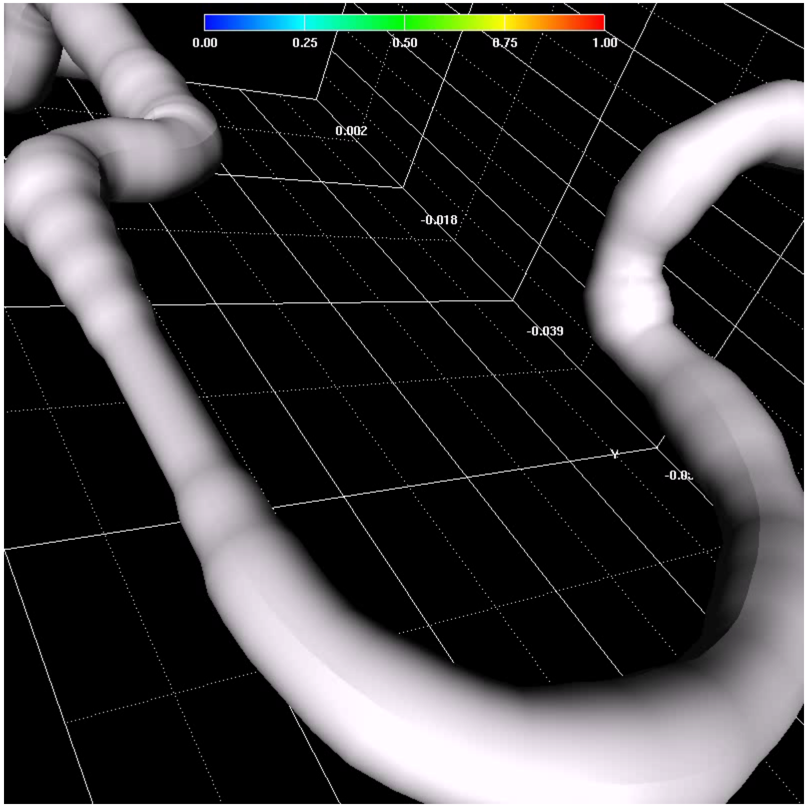
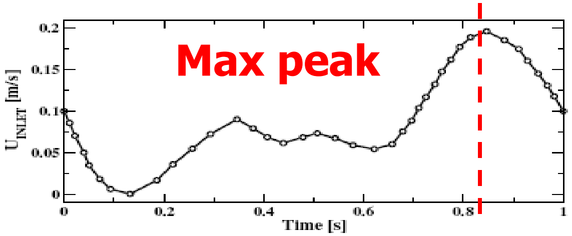
Pulsating simulations (healthy and 50% stenotic RC artery):







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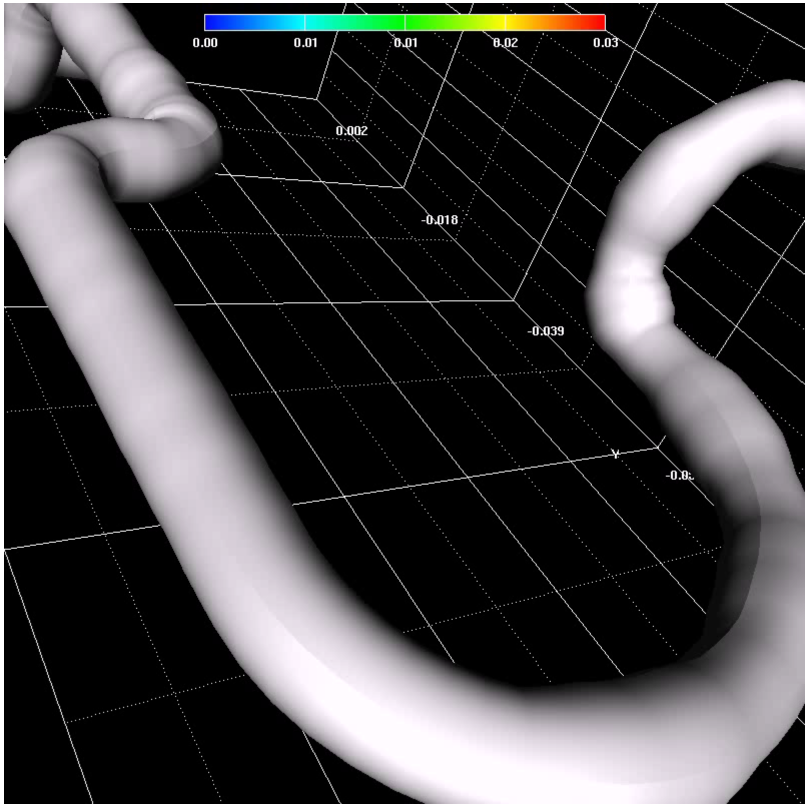
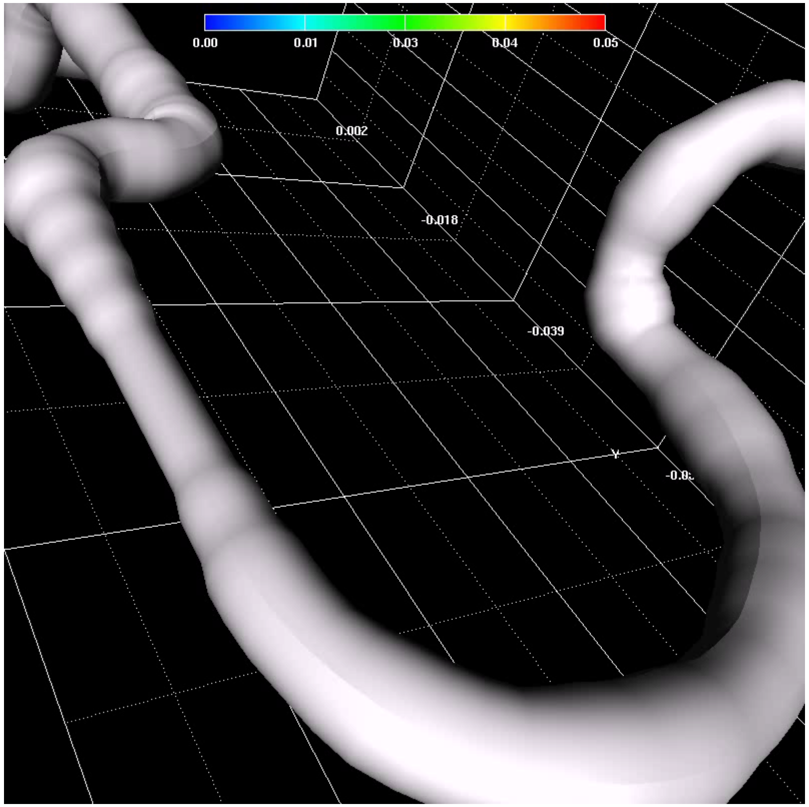
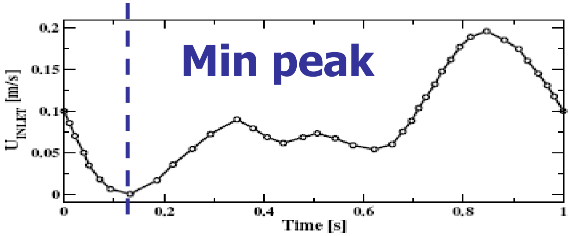
Pulsating simulations (healthy and 50% stenotic RC artery):







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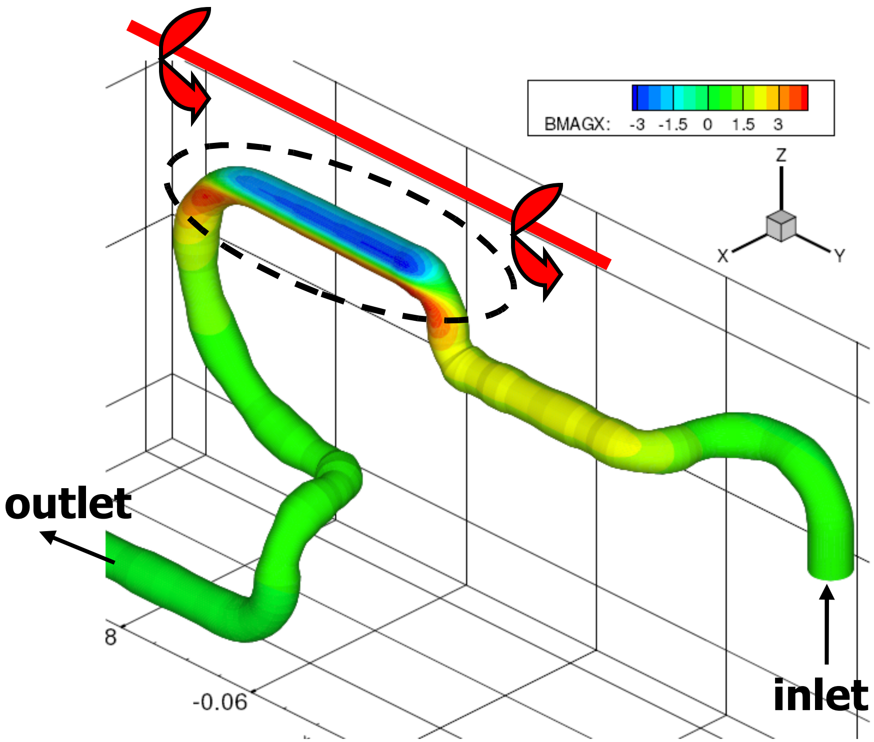
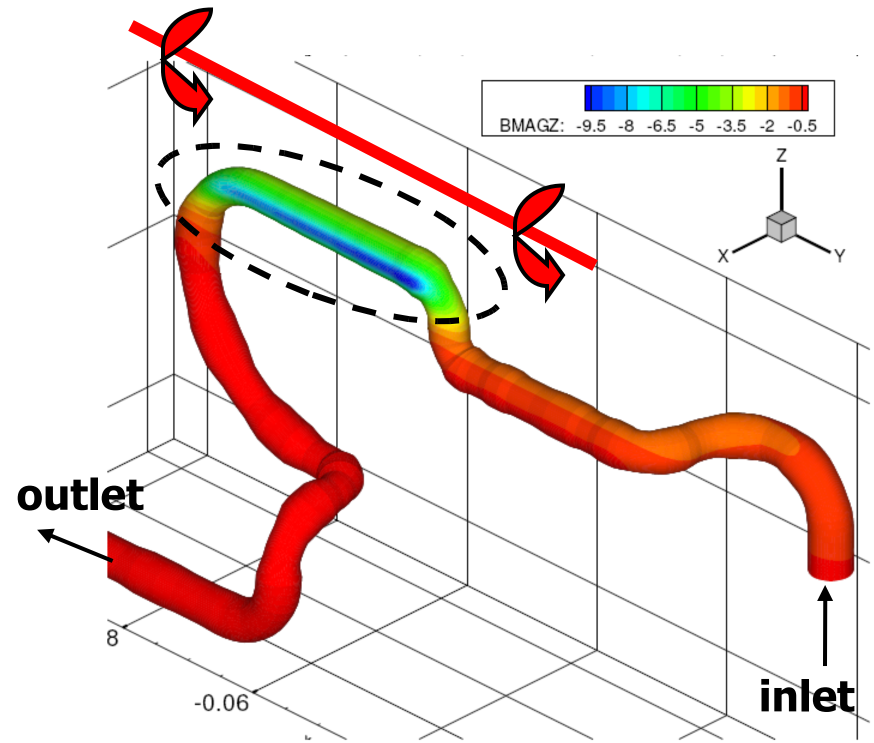
Numerical simulations (healthy artery: 0% stenotic) – steady

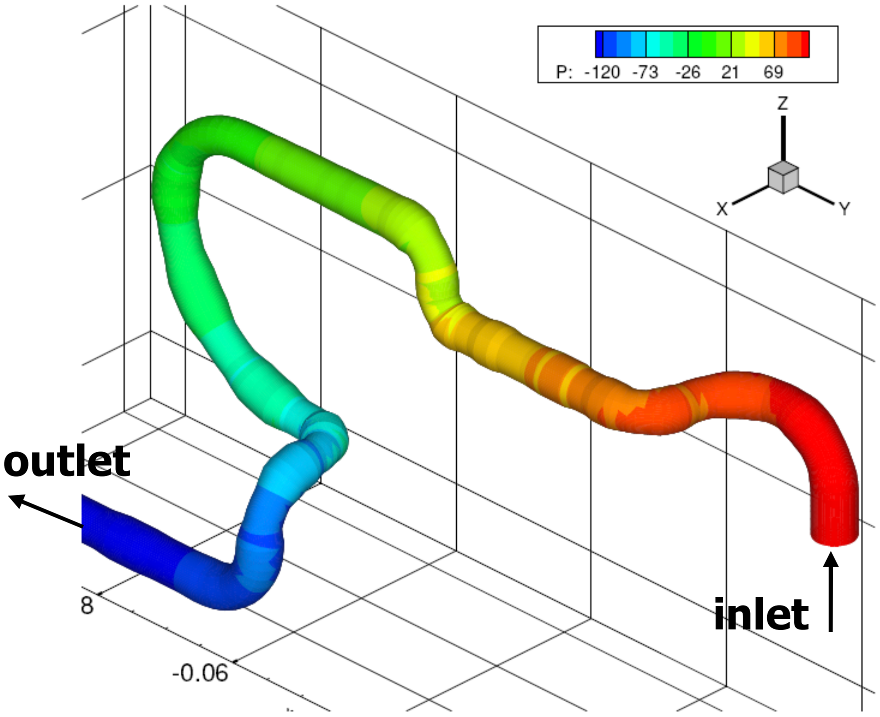


-Bx magnetic field component-

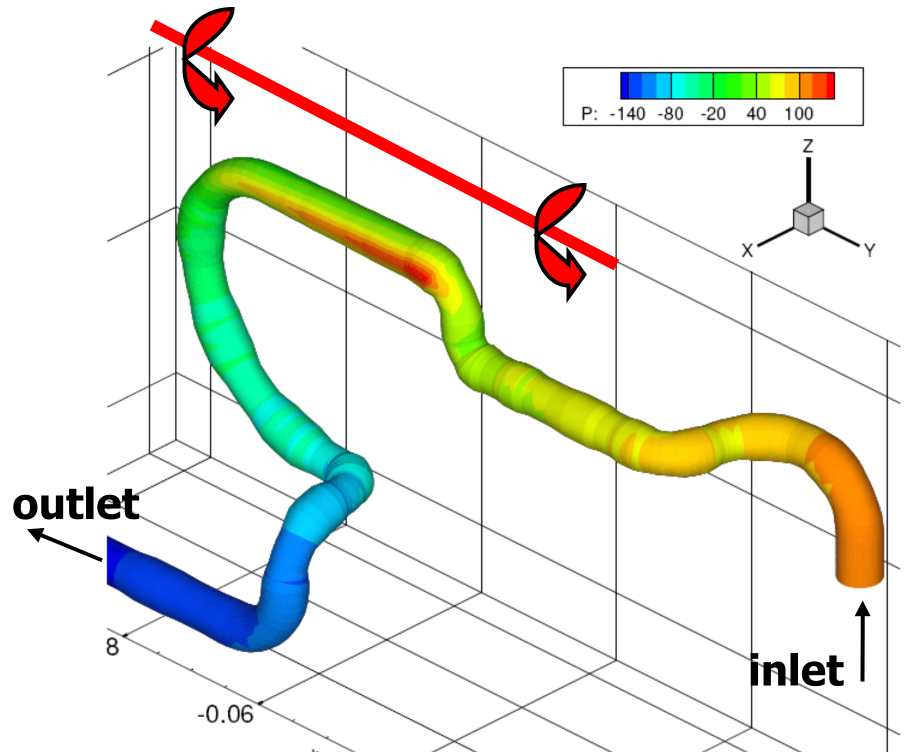


-Bz magnetic field component-

Numerical simulations (healthy artery: 0% stenotic) – steady



-magnetic field off-



-magnetic field on-

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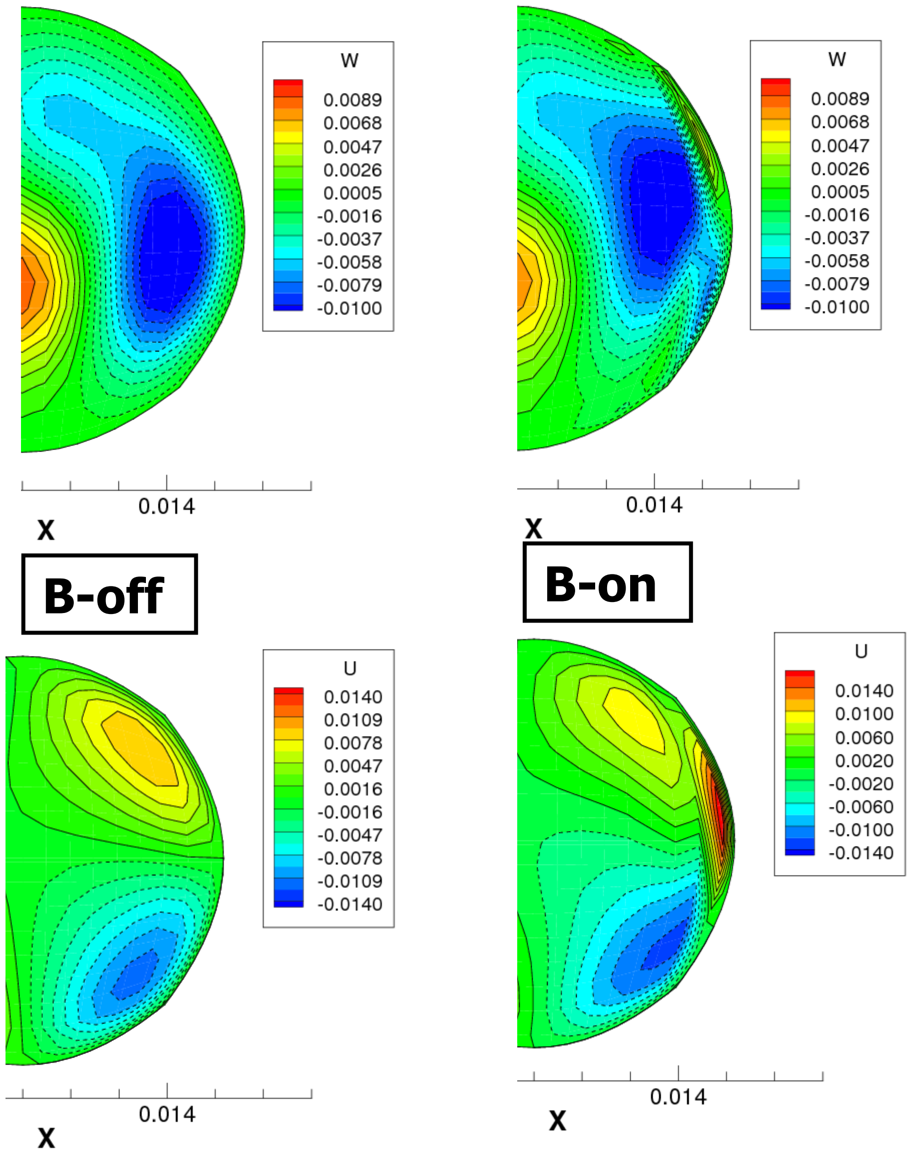

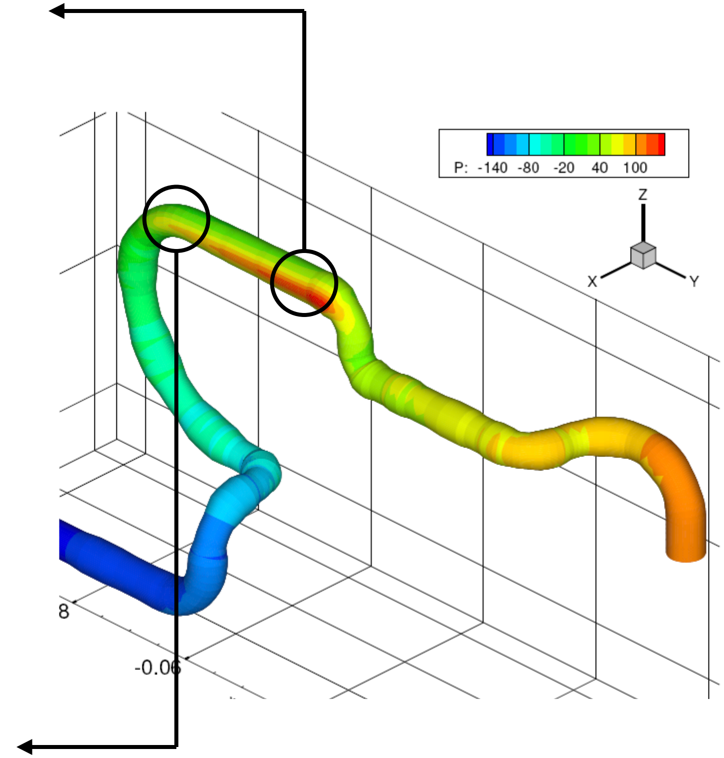

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Conclusions and outlook:

-A comprehensive mathematical model for blood flow subjected to strong non-uniform external magnetic fields derived (fluid flow/electromagnetism interactions)

-An extensive literature survey performed in order to collect physical properties of blood (both dynamical and electrical properties)

- Effects of imposed magnetic field on blood flow patterns clearly demonstrated for steady and pulsating flows in generic and realistic blood vessels geometries

- Future studies: non-linear magnetisation model (fluid-flow/biochemistry coupling)

- Future studies: non-Newtonian effects (pulsating cycles)

- Future studies: multi-branching blood vessels + fluid/structure interactions