



Center for Biomedical Computing

# FEniCS: An Attempt to Combine Simplicity, Generality, Efficiency and Reliability

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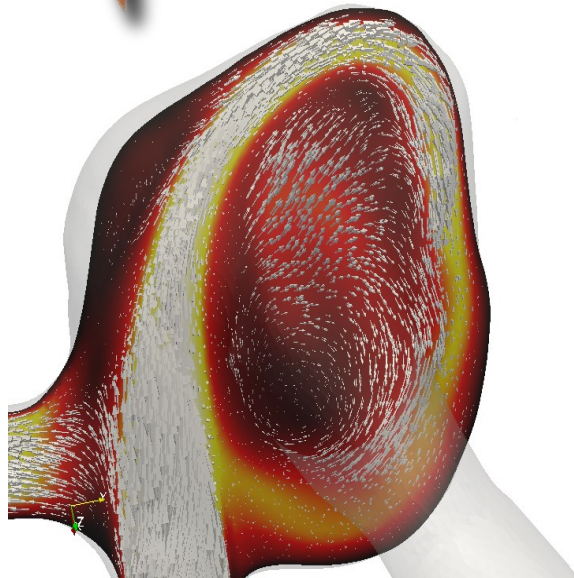
Joint work with Kristian Valen-Sendstad, Martin Alnæs, Mikael Mortensen, Anders Logg, Garth Wells, and Hans Petter Langtangen



# Outline



The use of the finite element library FeniCS exemplified with a few simple problems



FeniCS in use patient-specific simulations of blood flow in cerebral aneurysm

# Part I: The Finite element library FEniCS



FEniCS combines:

- \* high-level scripting techniques (Python)
- \* symbolic mathematics
- \* automatic differentiation
- \* code generation (low level C++ for efficient computations via a domain specific language and compiler)
- \* state-of-the-art linear algebra (PETSc, Trilinos, uBLAS, MTL)

FEniCS is open source

Focus is put on user-friendliness, generality and efficiency



# Simple example: Poisson equation

## Mathematical formulation

Find  $u$  such that for all  $v$

$$a(u, v) = L(v)$$

where

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx$$

$$L(v) = \int_{\Omega} f v \, dx$$

## Corresponding code

```
u = TrialFunction(V)
v = TestFunction(V)

a = dot(grad(u), grad(v))*dx
L = f*v*dx

problem = VariationalProblem(a, L)
u = problem.solve()
```

# The generated code is typically many times faster than corresponding hand-written quadrature code

Order	Quadrilateral					Hexahedron			
	1	2	3	4	5	1	2	3	4
Timescale (in $\mu s$ )	0.073	0.24	0.52	1.2	3.2	0.36	2.3	20.6	75.8
SFC (analytic)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
SFC (quadrature)	4.5	11.7	26.1	41.7	68.5	7.8	52.2	83.8	209.6
Deal.II	31.6	52.8	109.3	169.2	186.1	42.3	123.0	166.9	332.4
Diffpack	18.1	37.1	–	–	–	27.5	105.4	–	–

Table V. Time to compute the element tensor of the stiffness form for each order respectively on quadrilateral and hexahedron elements.

Alnæs and Mardal, TOMS 2010; Ølgaard and Wells TOMS 2010; Roghes, Kirby et.al. SISC 2009, Kirby and Logg, TOMS 2008,2007; The upcoming FENICS book



# Example 2: Poisson equation with discontinuous Galerkin

Find  $u$  such that for all  $v$

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx - \int_{\Gamma} \langle \nabla u \rangle \cdot \llbracket vn \rrbracket \, dS$$

$$- \int_{\Gamma} \llbracket un \rrbracket \cdot \langle \nabla v \rangle \, dS + \frac{\alpha}{h} \int_{\Gamma} \llbracket un \rrbracket \cdot \llbracket vn \rrbracket \, dS$$

$$L(v) = (f, v)$$

```

a = dot(grad(v), grad(u))*dx \
  - dot(avg(grad(v)), jump(u, n))*dS \
  - dot(jump(v, n), avg(grad(u)))*dS \
  + alpha/avg*dot(jump(v, n), jump(u, n))*dS \
L = f*v*dx

```

FENICS has support for many elements; continuous and discontinuous Lagrange, Nedelec, Raviart-Thomas, mixed methods etc.



# Hyper elasticity (Fung's law)

$$F = I + (\nabla u)$$

$$C = F^T : F$$

$$E = (C - I)/2$$

$$\psi = \frac{\lambda}{2} \text{tr}(E)^2 + K \exp(\text{inner}(E, E))$$

$$P = \frac{\partial \psi}{\partial E}$$

$$L = \int_{\Omega} P : (\nabla v) dx$$

$$J = \frac{\partial L}{\partial u}$$

- $u$  - unknown displacement
- $v$  - test function
- $I$  - identity matrix
- $A$ ,  $\lambda$  and  $K$  are material parameters
- $L$  - system of nonlinear equations
- $J$  - corresponding Jacobian

```
U = Function(V)

v = TestFunction(V)
u = TrialFunction(V)

lamda = Constant(1.0)
A = Expression (((('1.0 + x[0]', '0.3'), ('0.3', '2.3'))))
K = Constant(1.0)
n = U.cell().n

I = Identity(U.cell().d)
F = I + grad(U)
J = det(F)

C = F.T*F
E = (C-I)/2
E = variable(E)

psi = lamda/2 * tr(E)**2 + K*exp(inner(A*E,E))
P = F*diff(psi, E)
a_f = psi*dx
L = inner(P, grad(v))*dx
J = derivative(F, U, u)

A = assemble(J)
```

# Hyperelasticity VS Linear Elasticity Efficiency Tests

$N$	100	200	400
$J_L, p = 1$	0.08	0.27	1.04
$J_L, p = 2$	0.36	1.41	5.45
$J_F, p = 1$	0.33	0.84	3.36
$J_F, p = 2$	0.68	2.26	8.55

Table 15.1: Comparison of the time (in seconds) for computing the Jacobian matrix for the two elasticity problems on a  $N \times N$  unit square mesh for linear ( $p = 1$ ) and quadratic elements ( $p = 2$ ).

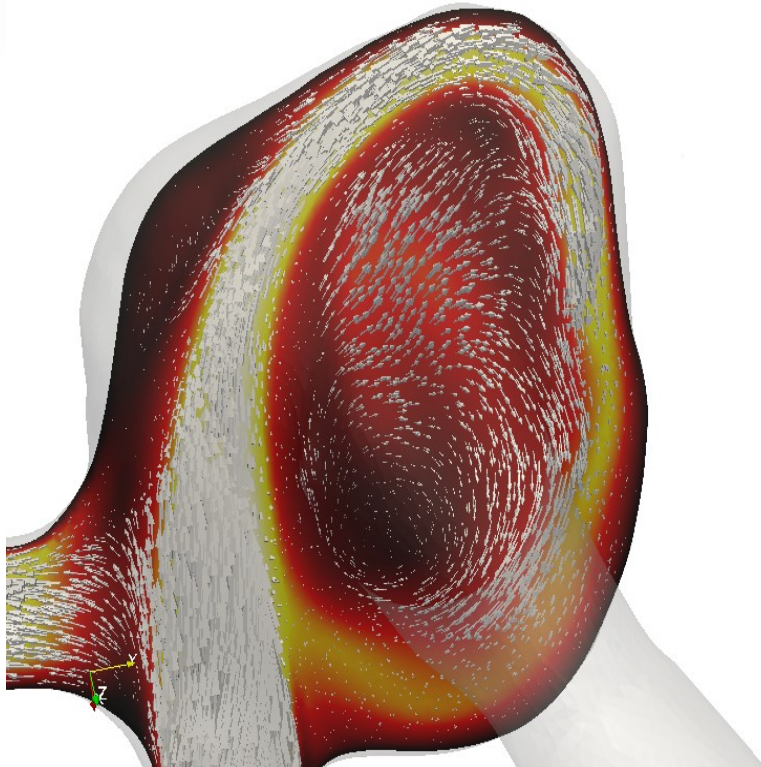
Testing the efficiency of the assembly process for the nonlinear Fung type elasticity problem reveals that it is only 2-3 times slower than linear elasticity!!!

Much better than we expected!!

UFL: see Alnæs: <https://launchpad.net/ufl>, and the upcoming book.



# Part II: Using FEniCS to study cerebral blood flow



```
# Tentative velocity step
U = 0.5*(u0 + u)
F1 = (1/k)*inner(u - u0, v)*dx \
    + inner(grad(u0)*n0, v)*dx \
    + inner(sigma(U, p0, nu), epsilon(v))*dx \
    + inner(p0*n, v)*ds \
    - beta*nu*inner(grad(U).T*n, v)*ds \
    - inner(f, v)*dx
a1 = lhs(F1)
L1 = rhs(F1)

# Pressure correction
a2 = inner(grad(p), grad(q))*dx
L2 = inner(grad(p0), grad(q))*dx \
    - (1.0/k)*div(u1)*q*dx

# Velocity correction
a3 = inner(u, v)*dx
L3 = inner(u1, v)*dx - k*inner(grad(p1 - p0), v)*dx
```

Incremental pressure correction

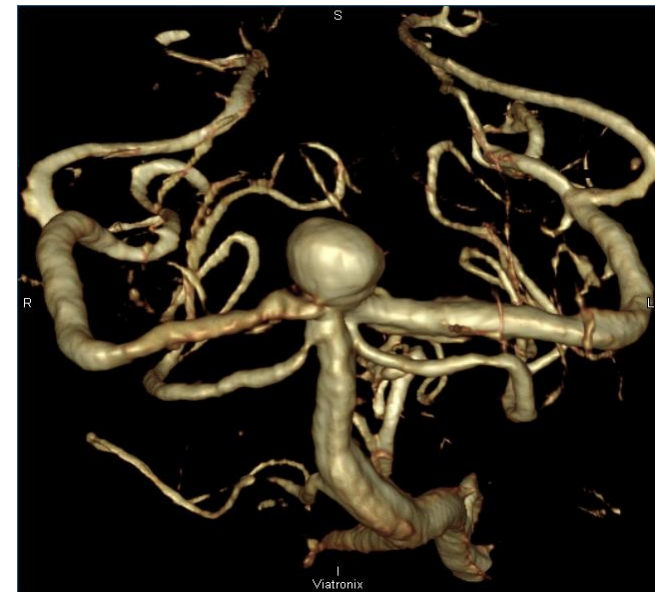
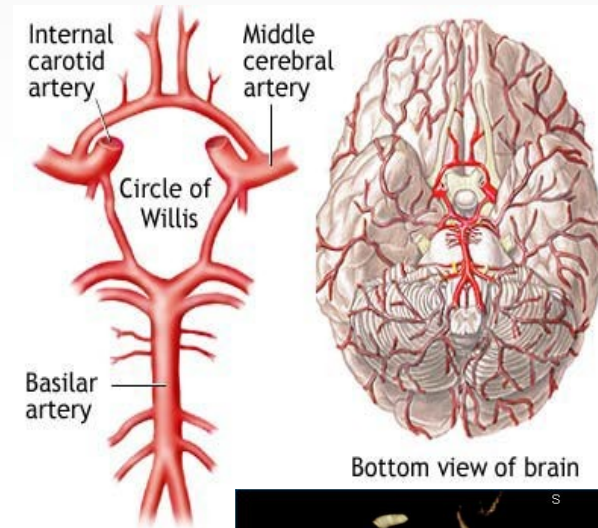
# The circle of Willis

The circle of Willis is the brain's main supplier of blood

It connects the carotid and vertebral arteries into a network that ensures a robust and stable blood supply to the brain

Unfortunately, aneurysms are often found in the circle of Willis (1-6%)

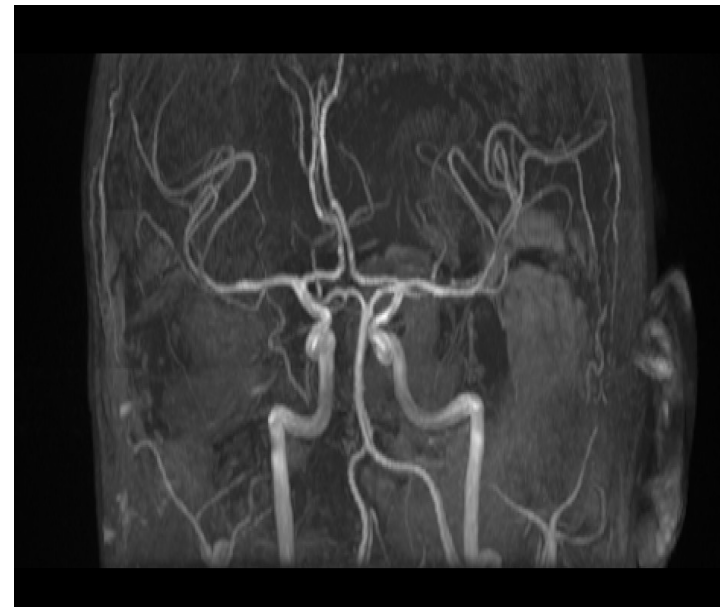
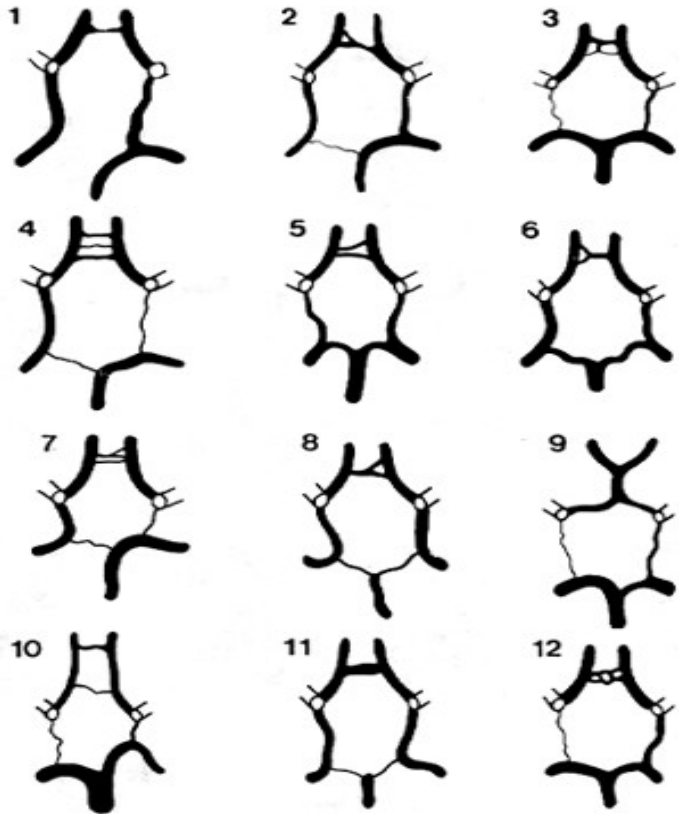
Aneurysms may rupture and cause a stroke  
Annual risk is assumed to be ~ 1%



# What causes aneurysm development and rupture?

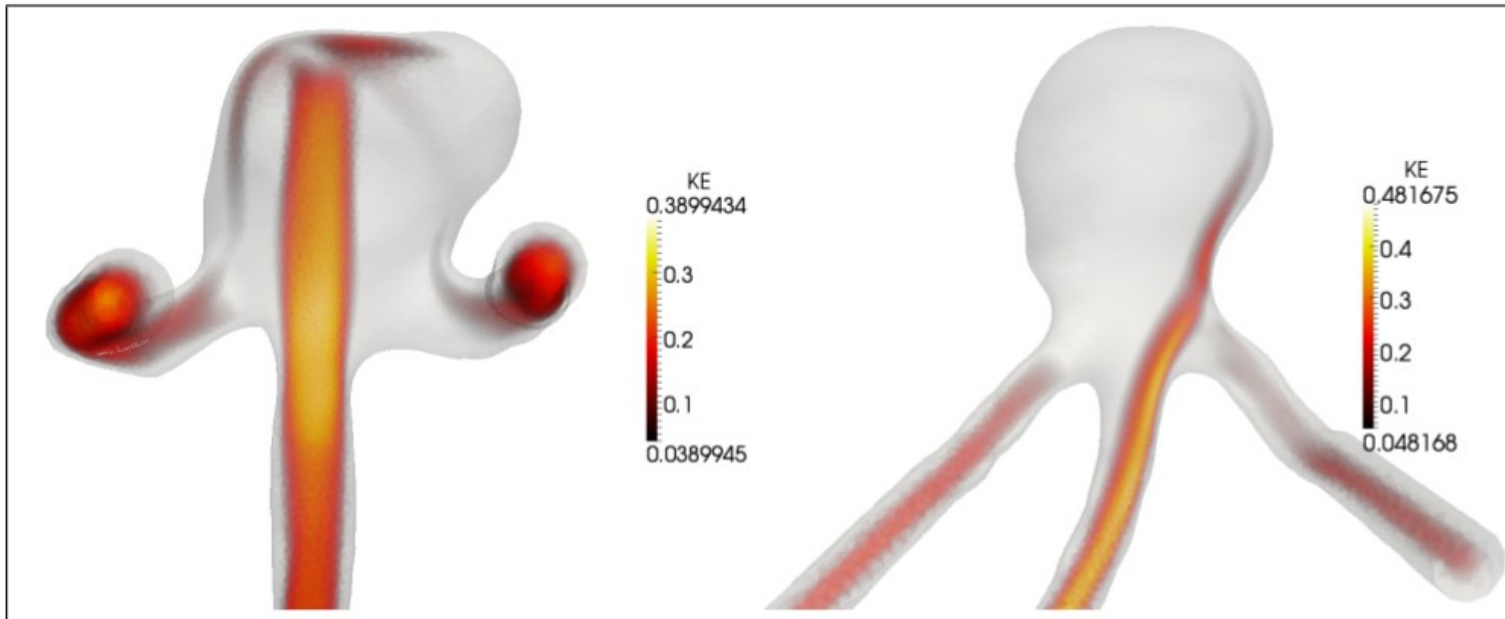
There are great variations in anatomy Eg only 50% have a well-balanced circle

Our hypothesis: Abnormal anatomy  
-> abnormal flow



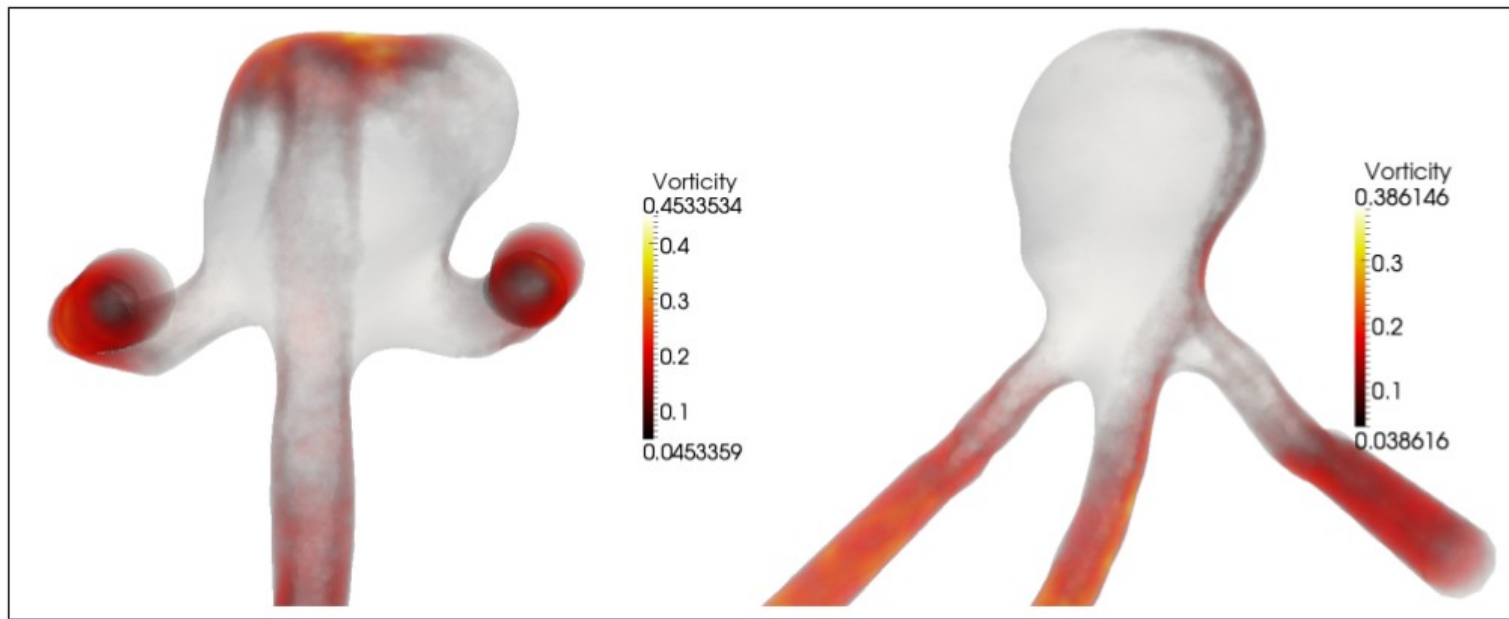
# Movie

# Some aneurysm focus the flow and kinetic energy



Volume visualization of kinetic energy in two different aneurysms. Only the upper 10% of the kinetic energy is shown. [Valen-Sendstad, Mardal et. al., submitted to Stroke]

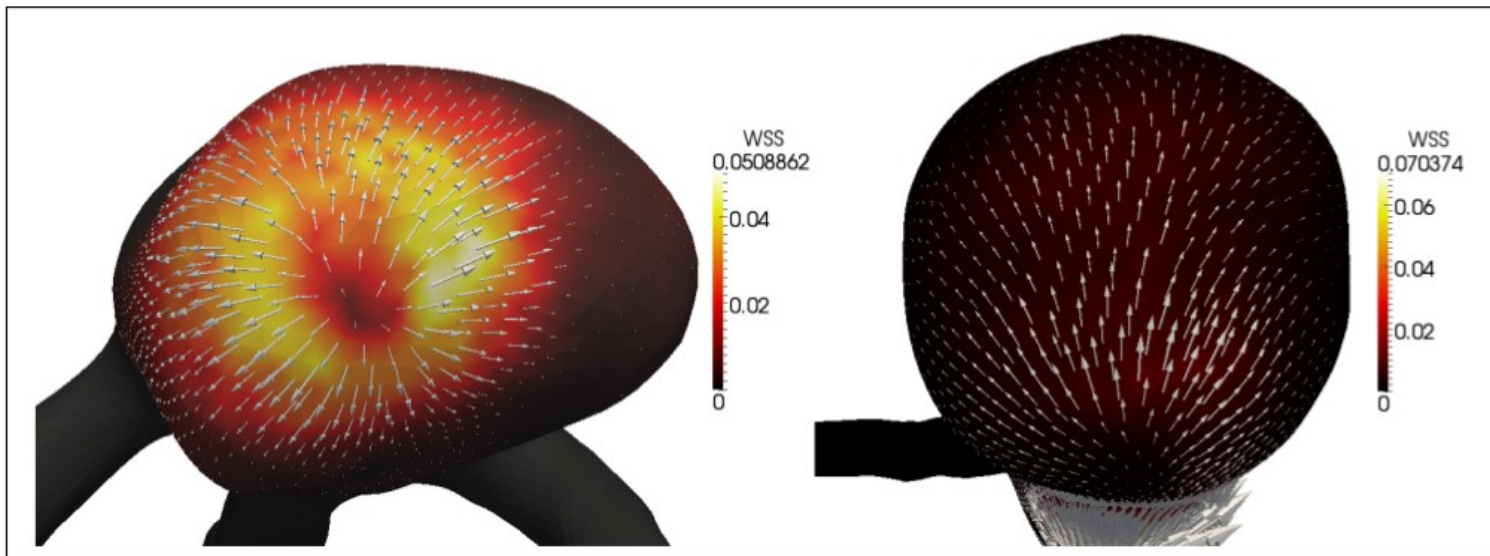
# Vorticity is produced as the kinetic energy is focused



Volume visualization of vorticity in two different aneurysms. Only the upper 10% of the vorticity is shown. [Valen-Sendstad, Mardal et. al., submitted to Stroke]



# High values of kinetic energy and vorticity are linked to large local variations wall shear stress



Visualization of the wall shear stress in the same aneurysms, but seen from different angles. Notice the stagnation zone.

# A patient study with 12 patients reveals differences between the ruptured and unruptured aneurysms

	Not Ruptured [ $\mu \pm \sigma$ ]	Ruptured [ $\mu \pm \sigma$ ]	Difference[%]	P-value
Height [ $mm$ ]	$5.25 \pm 2.01$	$5.92 \pm 2.97$	13%	-
Diameter [ $mm$ ]	$4.79 \pm 1.88$	$5.23 \pm 2.80$	9%	-
Volume [ $mm^3$ ]	$110.26 \pm 100.10$	$168.48 \pm 173.98$	63%	-
$KE_{\max}[\frac{mm^2}{ms^2}]$	$0.094 \pm 0.038$	$0.16 \pm 0.036$	70%	<b><math>p &lt; 0.005</math></b>
$KE_{\rho}[\frac{1}{ms^2mm}]$	$0.000128 \pm 0.00013$	$0.00031 \pm 0.00040$	242%	$p < 0.2$
$\omega_{\max}[\frac{1}{ms}]$	$0.091 \pm 0.0198$	$0.1615 \pm 0.0499$	77%	<b><math>p &lt; 0.01</math></b>
$\omega_{\rho}[\frac{1}{ms \cdot mm^3}]$	$0.00032 \pm 0.00029$	$0.00042 \pm 0.00049$	31%	$p < 0.35$
Max $\Delta P[\frac{g}{ms^2mm}]$	$0.1015 \pm 0.049$	$0.171 \pm 0.094$	68%	$p < 0.1$
Mean $\Delta P[\frac{g}{ms^2mm}]$	$0.047 \pm 0.0250$	$0.076 \pm 0.037$	62%	$p < 0.1$
WSS <sub>max</sub> $[\frac{g}{ms^2mm}]$	$0.0329 \pm 0.0089$	$0.0445 \pm 0.0162$	35%	$p < 0.1$
WSS <sub><math>\rho</math></sub> $[\frac{g}{ms^2mm^3}]$	$0.00016 \pm 0.0001$	$0.00024 \pm 0.00027$	50%	$p < 0.1$

Table 1: Table showing various measured and computed values for ruptured and unruptured aneurysms. The numbers are mean values ( $\mu$ ), plus/minus the standard deviation ( $\sigma$ ), and the difference between the mean values in percent. Right most columns shows the corresponding P-values using a Student-t test. Bold font numbers indicate statistical significance for  $p < 0.05$ .

# Movie

# Conclusion

Combining scripting techniques, symbolic mathematics, code generation, automatic differentiation and advanced linear algebra gives a user-friendly and efficient computational platform for solving PDE problems

A book about the FeniCS project is almost finished:

URL <https://launchpad.net/fenics-book>

A programable environment is really important when doing patient-specific simulations with a large number of patients

