JARA|HPC

Simulation and Optimization of Biomedical Devices.

Mike Nicolai

Jülich 7.5.2013

AN INITIATIVE OF RWTH AACHEN UNIVERSITY JÜLICH FORSCHUNGSZENTRUM

Contents

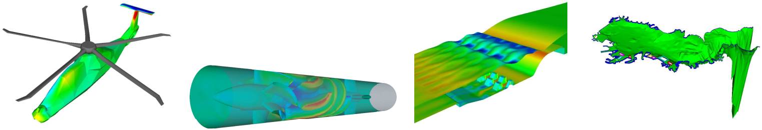
SimLab: Highly Scalable Fluids and Solids Engineering

- Goals:
  - Large scale CFD on massively parallel computers
  - Finding ways towards peta- and exascale computing
  - Porting and scaling of CFD applications and tools
  - Design of parallel PDE solvers (FEM and FVM)
  - Supporting researchers on HPC and CFD
- Know-How:
  - Finite Element Methods, Galerkin/Least-Squares (GLS), Discontinous Galerkin (DG) and Finite Volume Methods
  - Cartesian Grid-based methods and unstructured grid methods
  - Mesh partitioning and mapping
  - Automated parallel/distributed mesh generation
  - Shape optimization for fluids
  - Haemodynamics
  - etc.
- Applications:
  - Massively-parallel simulations,
  - Shape Optimization Framework,
  - Single-surface geometry representation.

SimLab: Highly Scalable Fluids and Solids Engineering

- Current HPC Projects:
  - Large Scale Mesh Decomposition
  - Tree-Code-Based Finite Volumes
  - Peta-Scaling of XNS (RWTH, Behr)
  - Peta-Scaling of ZFS (RWTH, Schröder)
- Current Support Projects
  - COPA-GT (CERFACS)
  - DIGITAL-X (DLR)
  - openFOAM on BGQ (Siemens)
- Current CFD Projects
  - Spatially Resolved Simulation of Packed Bed Chromatography (FZJ, Lieres)
  - Large-eddy simulations in support of accurate blood flow and blood damage simulations (RWTH, Behr)
  - Discontinuous Galerkin method for coupled aeroacoustics (RWTH, Schröder)

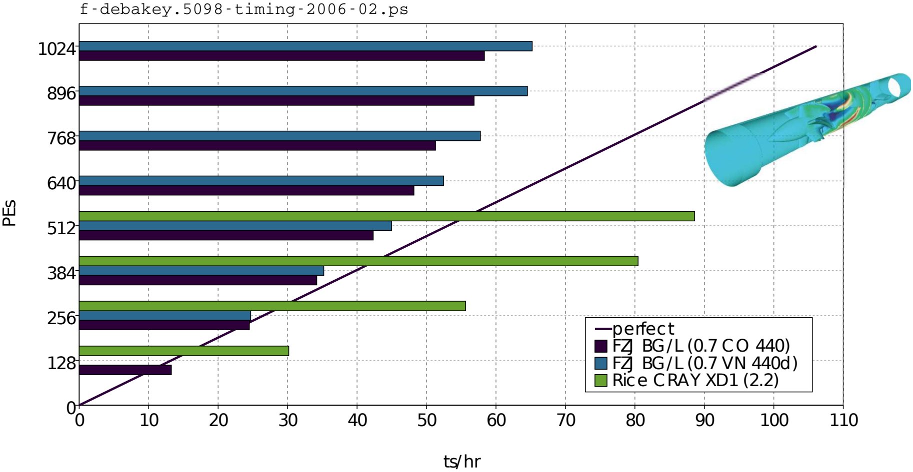
XNS Overview



(a) Boeing Sikorsky Comanche (b) DeBakey Blood-pump (c) Ohio (d) Tokio Bay

- The set of governing equations:
  - Advection-Diffusion
  - Incompressible Navier-Stokes
  - Compressible Navier-Stokes
  - Shallow-Water Equations
- Highlights of XNS
  - Portable and parallel FE-code
  - Mesh update techniques
  - Viscoelastic fluids
  - Large-Eddy Simulations
  - Free surface flows
  - Discretization: (fully implicit) space-time or semi-discrete
  - Shape Optimization

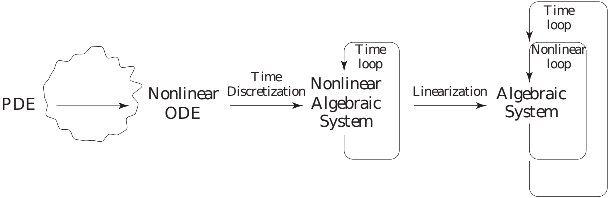
Simulation performance Blue/Gene 2006



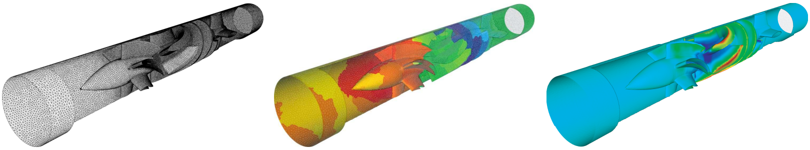
- Expected scaling up to 2048 to 4098 PEs.

Parallel Linear Solver

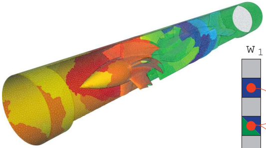
- PDE solver heavily depends on solutions of linear equation systems:

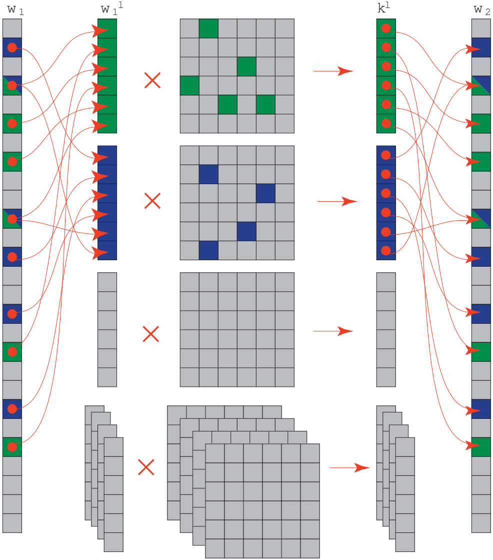


- GMRES solver, (block-)diagonal and ILU preconditioning,
- Utilizing a distributed vector-matrix multiplication.

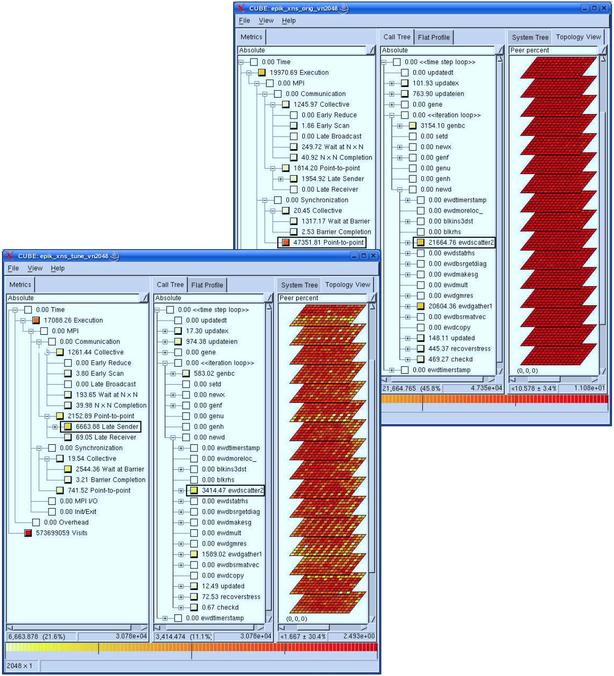


Distributed Vector-Matrix Multiplications



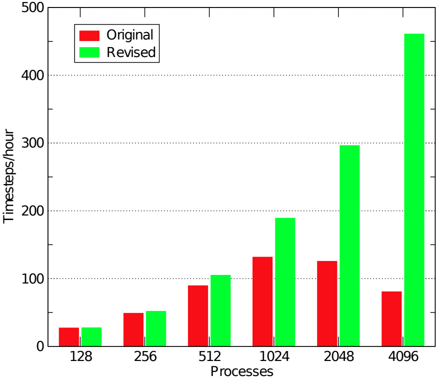


Scalasca

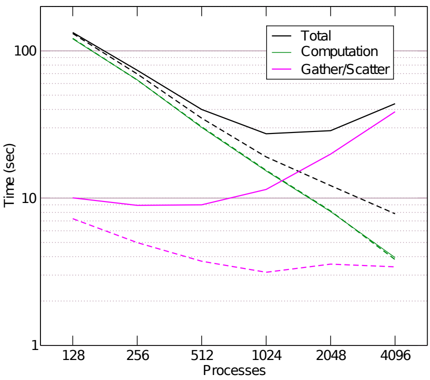


CUBE: epik_xns_orig_vn2048
File View Help
Metrics
Call Tree Flat Profile
System Tree Topology View
Absolute
Absolute
Peer percent
0.00 Time
19970.69 Execution
0.00 MPI
0.00 Communication
1245.97 Collective
0.00 Early Reduce
1.86 Early Scan
0.00 Late Broadcast
249.72 Wait at N x N
40.92 N x N Completion
1814.20 Point-to-point
1954.92 Late Sender
0.00 Late Receiver
0.00 Synchronization
20.45 Collective
1317.17 Wait at Barrier
2.53 Barrier Completion
47351.81 Point-to-point
0.00 <<time step loop>>
0.00 updatedt
101.93 updatex
763.90 updateien
0.00 gene
0.00 <<iteration loop>>
3154.10 genbc
0.00 setd
0.00 newx
0.00 genf
0.00 genu
0.00 genh
0.00 newd
0.00 ewdtimerstamp
0.00 ewdmoreloc_
0.00 blkins3dst
0.00 blkrhs
21664.76 ewdscatter2
0.00 ewdstatrhs
0.00 ewdbsrgetdiag
0.00 ewdmakesg
0.00 ewdmult
0.00 ewdgmres
20604.36 ewdgather1
0.00 ewdbsrmatvec
0.00 ewdcopy
148.11 updated
445.37 recoverstress
469.27 checkd
0.00 ewdtimerstamp
(0, 0, 0)
21,664.765 (45.8%)
4.735e+04
<10.578 ± 3.4%
1.108e+01
CUBE: epik_xns_tune_vn2048
File View Help
Metrics
Call Tree Flat Profile
System Tree Topology View
Absolute
Absolute
Peer percent
0.00 Time
17088.26 Execution
0.00 MPI
0.00 Communication
1261.44 Collective
0.00 Early Reduce
3.80 Early Scan
0.00 Late Broadcast
193.65 Wait at N x N
39.98 N x N Completion
2152.89 Point-to-point
6663.88 Late Sender
69.05 Late Receiver
0.00 Synchronization
19.54 Collective
2544.36 Wait at Barrier
3.21 Barrier Completion
741.52 Point-to-point
0.00 MPI I/O
0.00 Init/Exit
0.00 Overhead
573699059 Visits
0.00 <<time step loop>>
0.00 updatedt
17.30 updatex
974.38 updateien
0.00 gene
0.00 <<iteration loop>>
583.02 genbc
0.00 setd
0.00 newx
0.00 genf
0.00 genu
0.00 genh
0.00 newd
0.00 ewdtimerstamp
0.00 ewdmoreloc_
0.00 blkins3dst
0.00 blkrhs
3414.47 ewdscatter2
0.00 ewdstatrhs
0.00 ewdbsrgetdiag
0.00 ewdmakesg
0.00 ewdmult
0.00 ewdgmres
1589.02 ewdgather1
0.00 ewdbsrmatvec
0.00 ewdcopy
12.49 updated
72.53 recoverstress
0.67 checkd
0.00 ewdtimerstamp
(0, 0, 0)
6,663.878 (21.6%)
3.078e+04
3,414.474 (11.1%)
3.078e+04
<1.667 ± 30.4%
2.493e+00
2048 x 1

Simulation performance JUGENE 2008



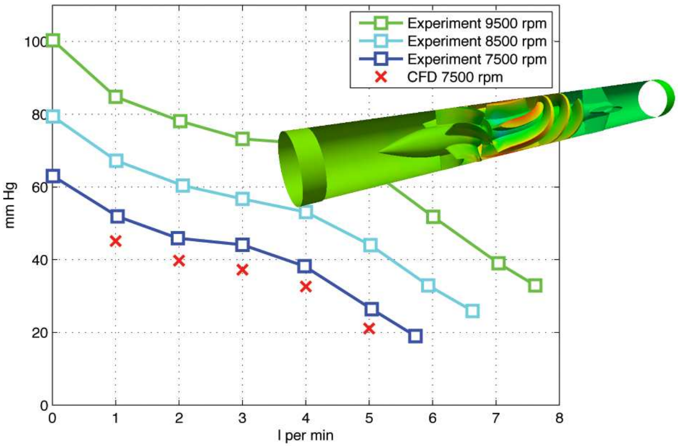
(a) Overall simulation performance



(b) Breakdown by solver component

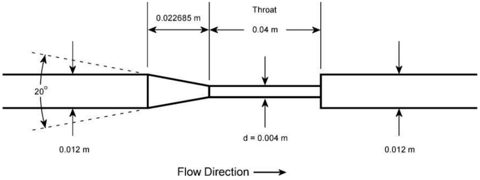
Validation DeBakey Blood Pump

- Experimental results provided by MicroMed,
- CFD validation done with XNS flow solver:

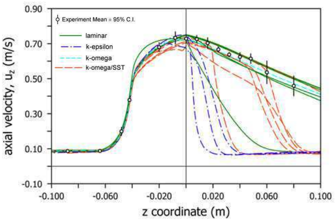


FDA's 'Critical Path' Initiative

- Round-Robin Study with 28 participating research groups.
- Simple Geometry:

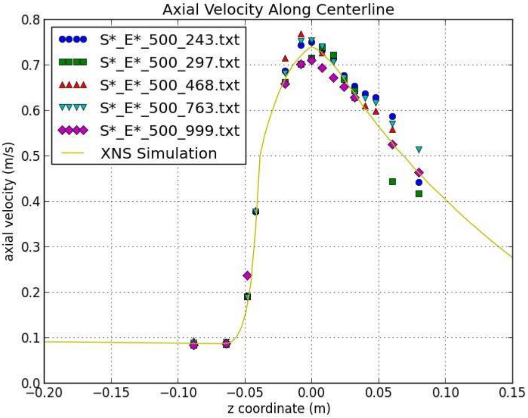


- Centerline velocity at Re = 500 from [Stewart 2012] :



FDA's 'Critical Path' Initiative

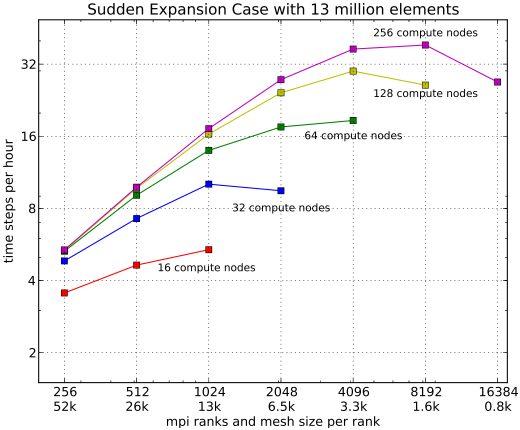
- Centerline velocity at Re = 500 with XNS:



- Tetrahedral mesh with 13 million elements

FDA's 'Critical Path' Initiative

- Scalability on JuQueen:



- BG/Q has four floating point units per core,
- XNS is able to exploit them efficiently.

Spatially Resolved Chromatography Simulations

- Important unit operation for compounds separation:

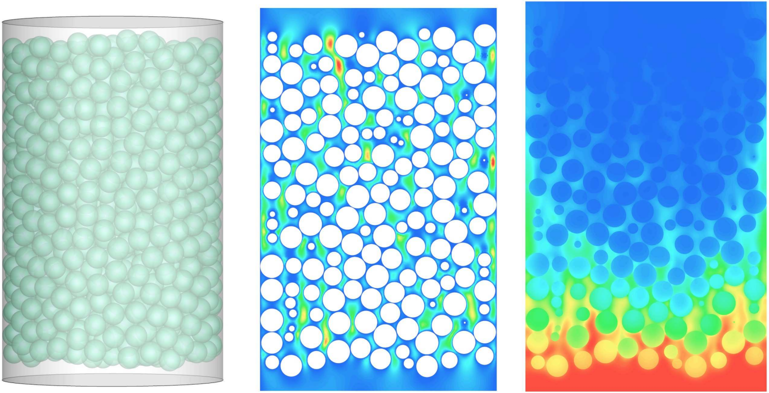
(a) Industrial scale

(b) Laboratory scale

- Collaboration project with Eric von Lieres (FZJ, IGB-1 Biotechnology),
- Common homogeneity assumptions not appropriate at small scales,
- Status Feb. 2012 : 750 beads simulation (flow only),
- Status Feb. 2013 : 8000 beads simulation (flow + mass-transfer).
- New model for scale-up (laboratory scale to industrial scale) needed.

Spatially Resolved Chromatography Simulations

- Example simulation with 1257 randomly packed beads:

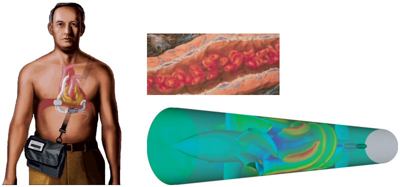


(a) Geometry (b) Flow profile (c) Trans. mass transport

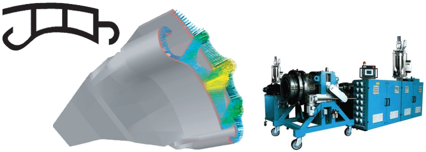
- Simulation contradicts homogeneity assumption.
- Current challenges are mesh generation and visualization.

Shape Optimization in an Engineering Context

- Shape optimization projects at CATS:



(a) blood pump design

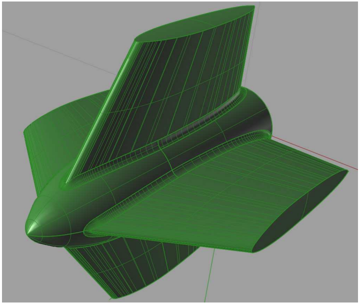


(b) extrusion die design

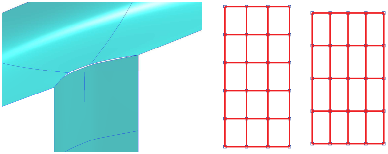
- Interface with CAD programs needed in two projects:
  - MicroMed Inc: Robust shape optimization for artifical blood pumps.
  - Excellence Cluster EXC 128: A2 Individualized production.
- Strong geometric constraints:
  - production limits,
  - design limits.
- Fundamental needs:
  - watertight model,
  - arbitrary topology possible,
  - NURBS compatible,
  - easy to parameterize.

T-Splines

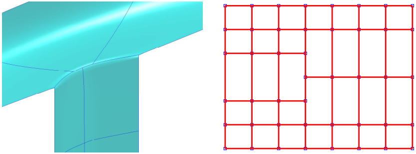
- Typical geometry in a CAD system:



- NURBS [Versprille 1975]:

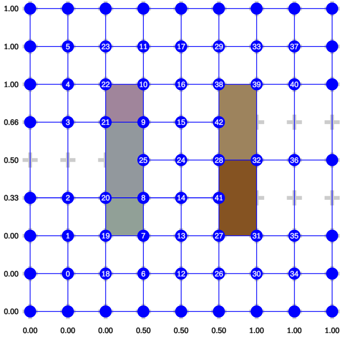


- T-spline [Sederberg 2003]:

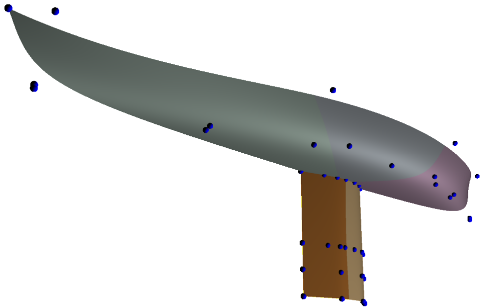


Model Generation: T-Splines

- T-spline spaces:



(a) index/parameter space



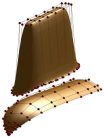
(b) physical space

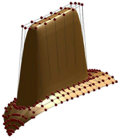
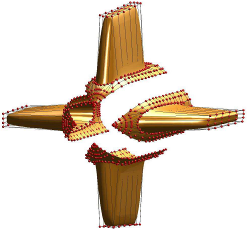
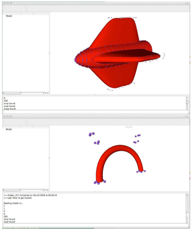
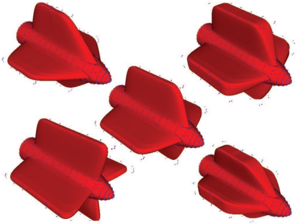
- T-spline surface is calculated by:

$$\mathbf{C}(\boldsymbol{\tau}) = \frac{\sum_i \beta_i \mathbf{P}_i B_i(\boldsymbol{\tau})}{\sum_i \beta_i B_i(\boldsymbol{\tau})}.$$

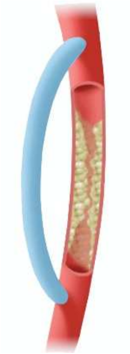
Model Generation: Toolchain

- Basic mesh generation:
  - Rhino™ for CAD model cleanup,
  - Pointwise™ for FE mesh generation,
  - file I/O with IGES.
- Shape parameterization with:
  - in-house Matlab™ toolbox (since 2007),
  - B-splines, T-splines (merge, glue and fit),
  - in-house graphical editor for the shape parameterization,
  - file I/O with IGES, STL and XML.
- Geometry kernel:
  - in-house Fortran 90 library (`shade`),
  - $\gamma(\boldsymbol{\alpha})$, $\frac{d\gamma(\boldsymbol{\alpha})}{d\boldsymbol{\alpha}}$,
  - file I/O via XML.



Shape Optimization Problem



- Problem: How to place a bypass?
- Minimize blood damage with

$$J(\mathbf{v}, \boldsymbol{\alpha}) = 2 \int_{\Omega_{\text{obs}}(\boldsymbol{\alpha})} \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) d\mathbf{x}$$

  as a simple hemolysis model.
- Navier-Stokes equations viewed by a fluid dynamicist:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \mathbf{u} - \mathbf{f} \right) - \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\mathbf{u}, p) = \mathbf{0}, \qquad \boldsymbol{\nabla} \cdot \mathbf{u} = 0 \qquad \text{on } \Omega.$$

- Navier-Stokes equations viewed as a generic state equation:

$$\mathbf{c}(\mathbf{u}, p; \mathbf{x}) = \mathbf{0}.$$

- Optimal shape design problem evaluates $\boldsymbol{\alpha} \in \mathcal{A}_{ad} \subset \mathbb{R}^n$:

$$\begin{aligned} \textit{minimize} \quad & J(\mathbf{u}, p, \boldsymbol{\alpha}), \\ \textit{subject to} \quad & \mathbf{c}(\mathbf{u}, p; \mathbf{x}(\boldsymbol{\alpha})) \text{ on } \Omega(\boldsymbol{\alpha}), \\ & \boldsymbol{\alpha} \in \mathcal{A}_{ad}. \end{aligned}$$

Shape Optimization Problem (cntd)

- Reformulated problem:

$$\begin{aligned} \textit{minimize} \quad & J(\mathbf{x}, \mathbf{v}, \boldsymbol{\alpha}), \\ \textit{subject to} \quad & \mathbf{0} = \mathbf{c}(\mathbf{v}; \mathbf{x}(\boldsymbol{\alpha})) \\ & \mathbf{0} = \mathbf{d}(\mathbf{x}(\boldsymbol{\alpha}); \boldsymbol{\gamma}(\boldsymbol{\alpha})) \\ \textit{on} \quad & \Omega = \Omega(\boldsymbol{\alpha}) \;\; \textit{with} \;\; \boldsymbol{\alpha} \in \mathcal{A}_{ad} \end{aligned}$$

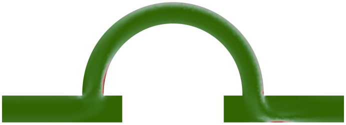
  with

$$\mathbf{v} = \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix}$$

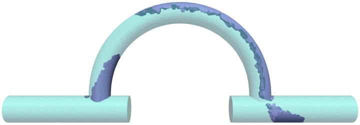
  for the incompressible Navier-Stokes states.
- Two approaches to solve this problem:
  - As one problem (SAND, fully-coupled),
  - As a coupled problem (NAND, black-box approach).
- Our way:
  - Solution as a coupled problem simplifies the use of existing solver,
  - Gradient-based approach.

Artificial graft optimization Re 200

- The initial shape ($J_{init} = 118$):



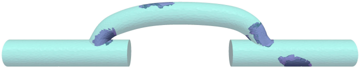
(c) Scalar shear rate range 0 .. 50



(d) Threshold > 20

- Optimal shape ($J_{opti} = 88.3$) with 24 parameters using the C^0-merge:

(e) Scalar shear rate range 0 .. 50



(f) Threshold > 20

Discussion

- Finite Elements for Fluids:
  - General FEM for flow problems,
  - Multi-physics.
- Issues in Massively-parallel Simulations:
  - Profiling,
  - Mesh generation
  - Mesh partitioning and mapping,
  - Visualization.
- Applications:
  - Massively-parallel simulations,
  - Shape Optimization Framework,
  - Single-surface geometry representation.