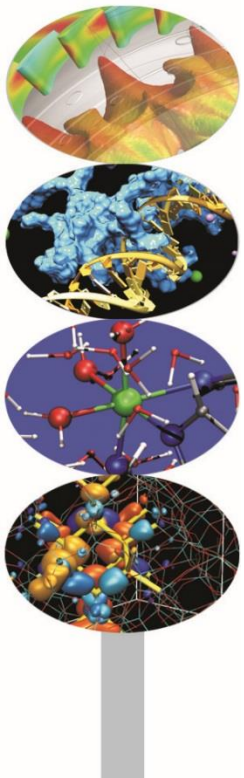
CINECA SCAI
SuperComputing Applications and Innovation

Comprehensive Heart Failure Center

Cineca TRAINING High Performance Computing 2016

Simulating Coronary Mass Transport with OpenFOAM



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Chair for Cellular and Molecular Imaging

April 7, 2016

PRACE

CINECA

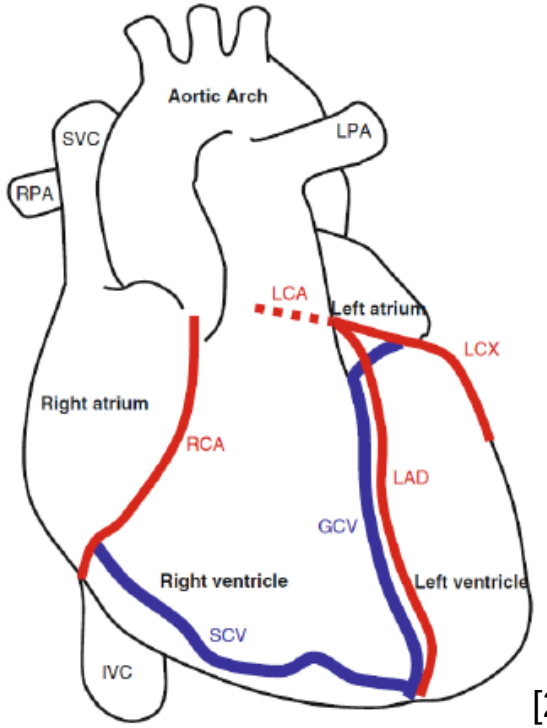
Overview

- Scientific Question
- Implementation in OpenFOAM
- Previous Results
- Scalability Testing
- Conclusion

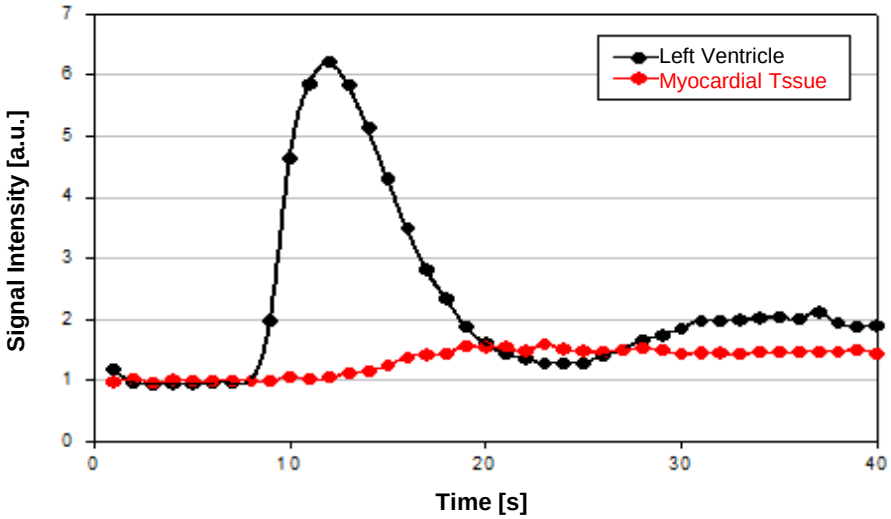
Scientific Question

Quantitative Perfusion MRI:

- Measure signal intensities in left ventricle and myocardial tissue
- Determine physiological parameters, i.e. myocardial blood flow, MBF between 0.590 and 2.050 ml/min/g tissue [1]



[2]

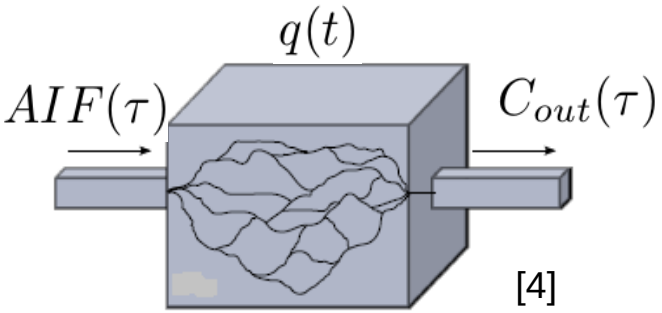


[3]

Scientific Question

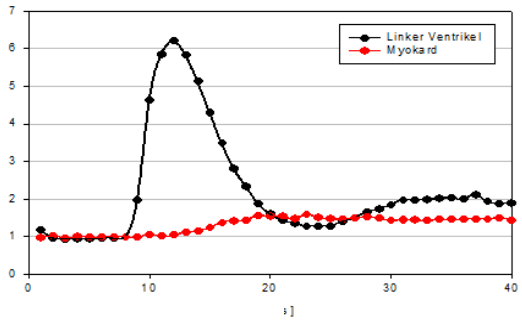
Determination of MBF:

Signal intensity: $$q(t) = MBF \int_0^t [AIF(\tau) - C_{out}(\tau)]\, d\tau$$



[4]

- $C_{out}(t)$ and $AIF(t)$ not measurable
  - ➡ Use of $AIF_{LV}(t)$



[3]

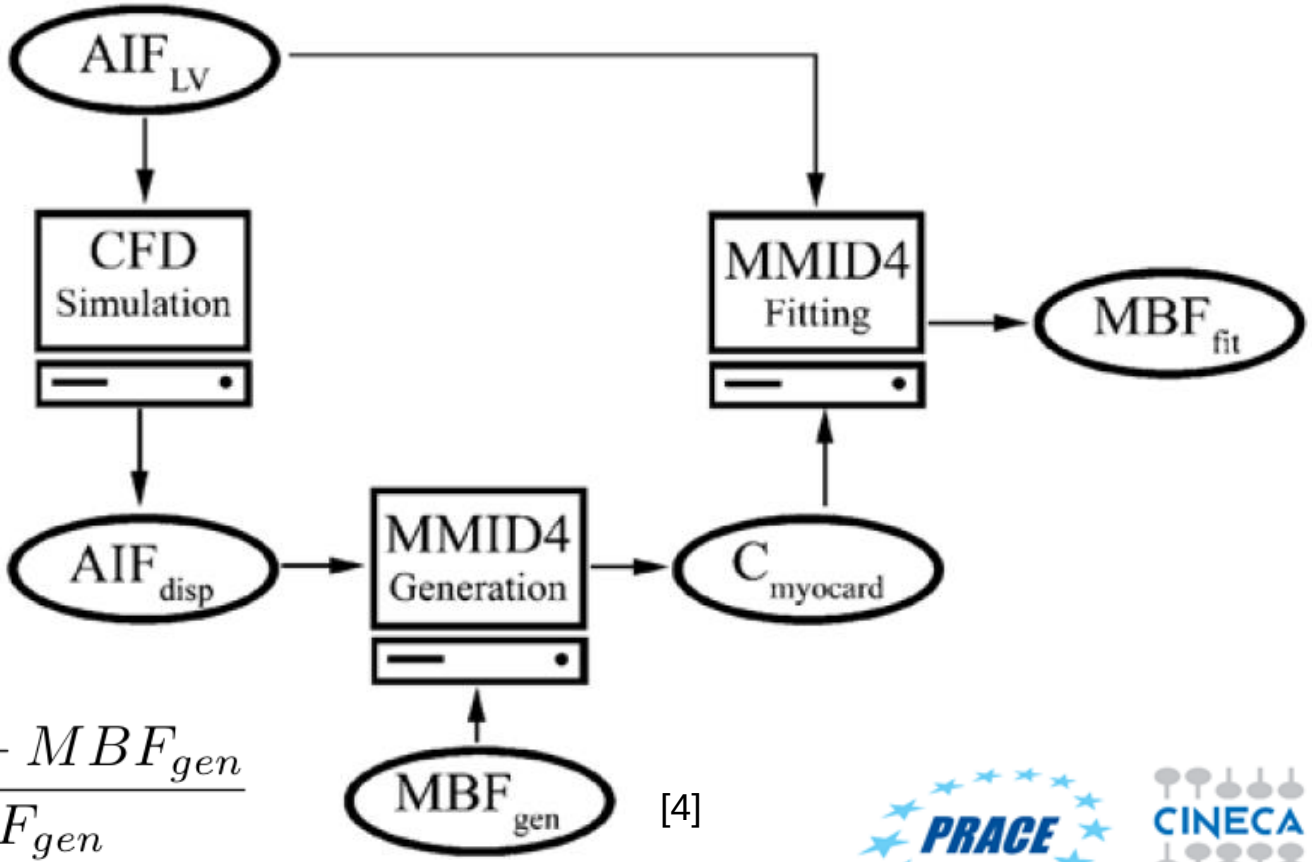
- Solve for MBF
  - Discrepancy in $AIF(t)$ ➡ Systematic error in MBF!

- CFD simulations to determine $AIF(t)$

[3] Julia Hamer et al., 2009. [4] K. Sommer et al., 2015.

Scientific Question

- Quantification of ΔMBF
- Calculation of MBF with MMID4 [5]



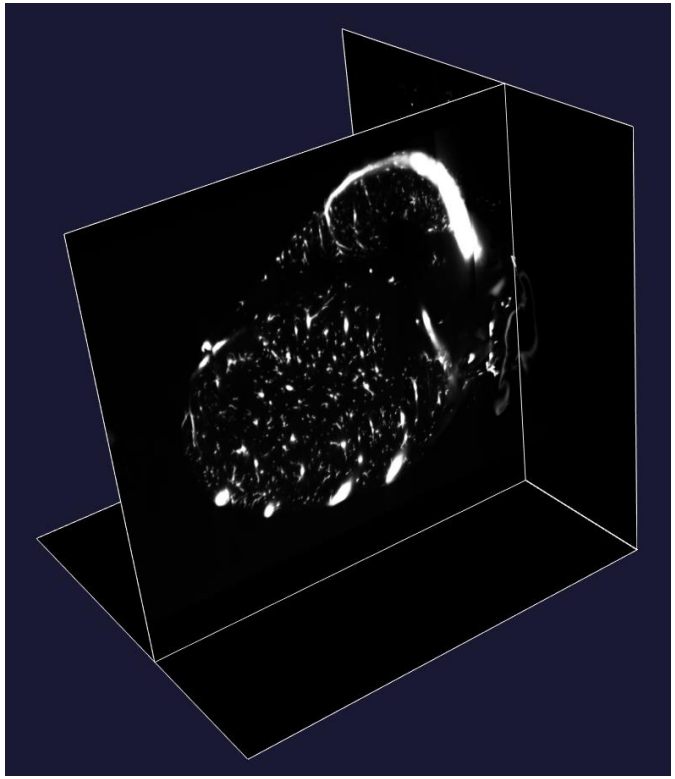
$$\Delta MBF = \frac{MBF_{fit} - MBF_{gen}}{MBF_{gen}}$$

[4]

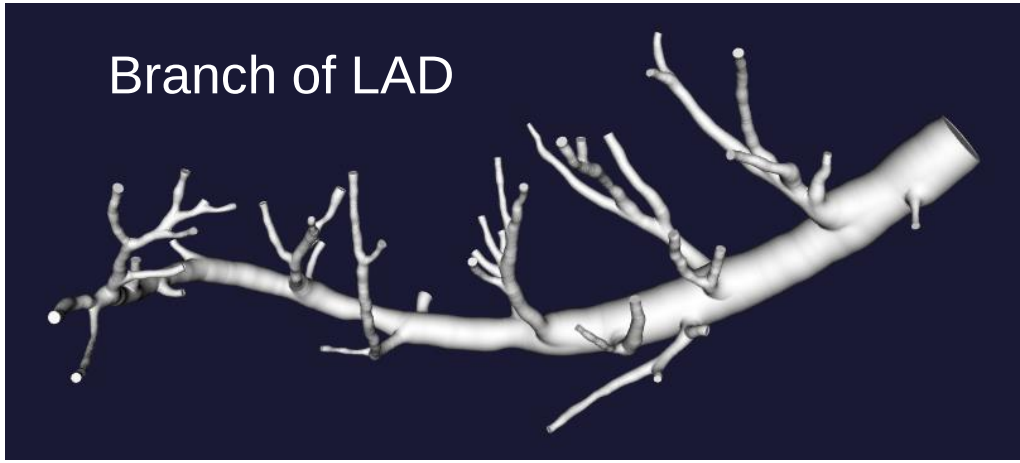
[4] K. Sommer et al., 2015.
[5] MMID4 Manual, Version 2.3, 1998.

Implementation in OpenFOAM

- Surface creation (e.g. VMTK [6])

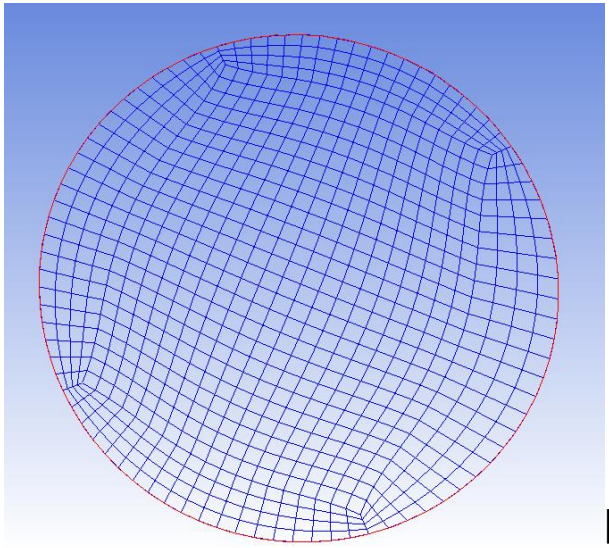


[7]

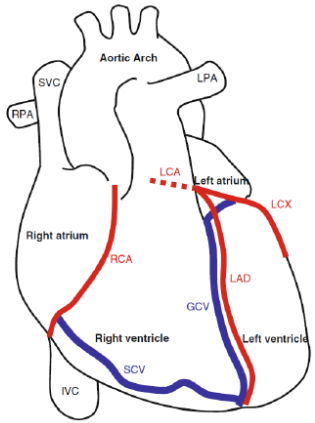


[8]

- Meshing with hexa-cells



[8]



[2]

[2] [2] Jack Lee et al., 2012.
[6] http://www.vmtk.org/, Version 1.2, 2015.
[7] M. Siebes et al., 2014.
[8] CHFC, 2015.

Implementation in OpenFOAM-2.2.2

Compute CA transport in 3D models of coronary vasculature:

Governing equations:

- Navier-Stokes-equation $$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \mu\Delta\mathbf{v} + \mathbf{b}$$
- Advection-Diffusion-equation $$\frac{\partial c}{\partial t} + \mathbf{v}\cdot\nabla c - D\Delta c = 0$$

2-Step procedure (with custom solvers):

1. Solve NSE, write fields to disk
2. Solve ADE (using written field ϕ)

Implementation in OpenFOAM

NSE solver:

- Based on OpenFOAM's `pisoFoam` solver
  - Periodicity criterion
  - Boundary conditions

- Boundary conditions
  - Inlet: $p = p(t)$ (oscillating)
  - Walls: $v = 0$ (no-slip)
  - Outlets: $Z_{outlet} = Z\left(r_{outlet}, r_{min}\right)$

  ⇨ $p_{outlet} = Z_{outlet} \cdot Q_{outlet}$ solved for each timstep

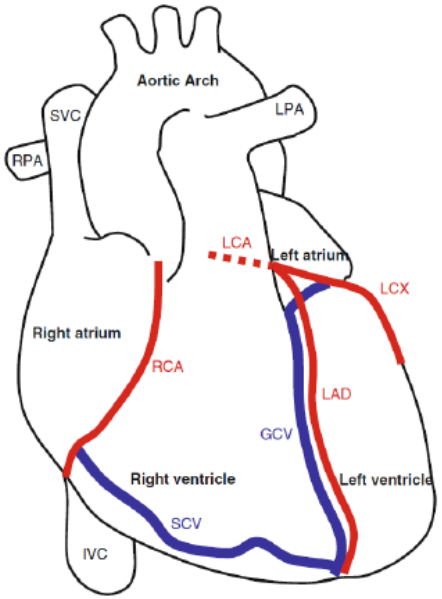
- Adjustable timestepping (Co < 0.5)

Implementation in OpenFOAM

ADE-Solver:

- Periodically reading flux field Φ
- Boundary Condition
  - Inlet: $c(t) = AIF_{LV}(t)$

Surface Model:



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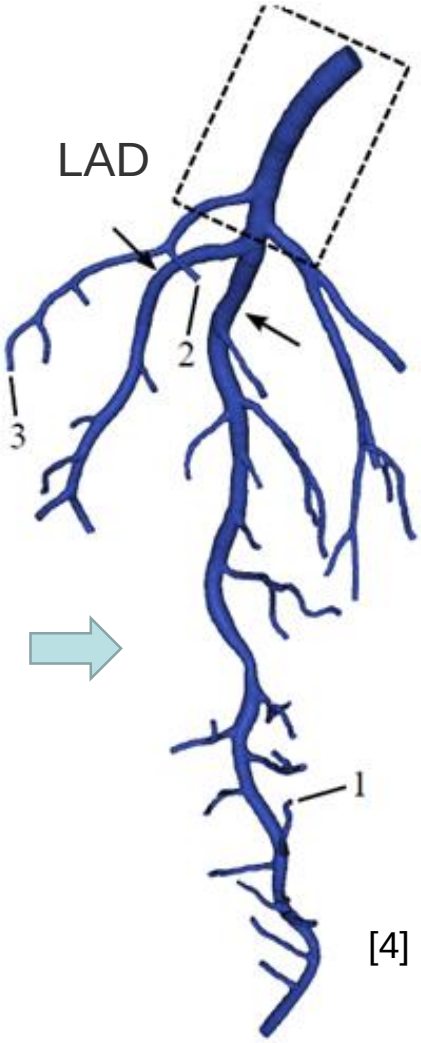


[4]

Previous Results

Simulation parameters: ~3.6 Mio Cells on 128 Cores

Solution of NSE:

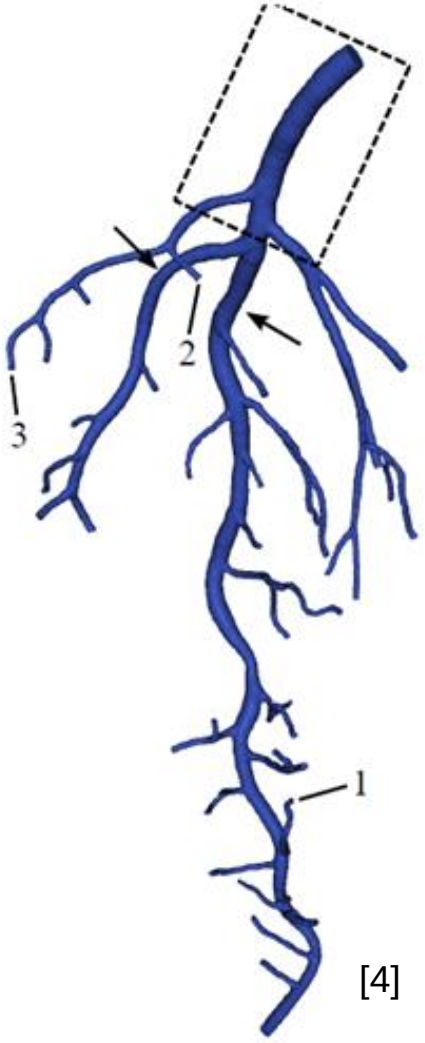
- Clocktime: ~7 days
- #files:

#cores * T_{cycle} / writeInterval

128 * 1s / 0.0001 s = ~12 Mio. Files

Solution of ADE:

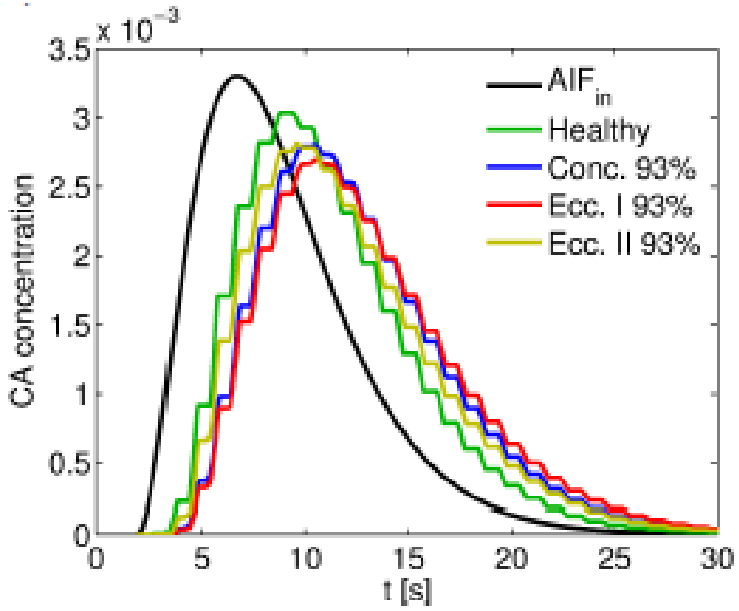
- Clocktime: ~1 day
- #files: ~2-3 Mio.

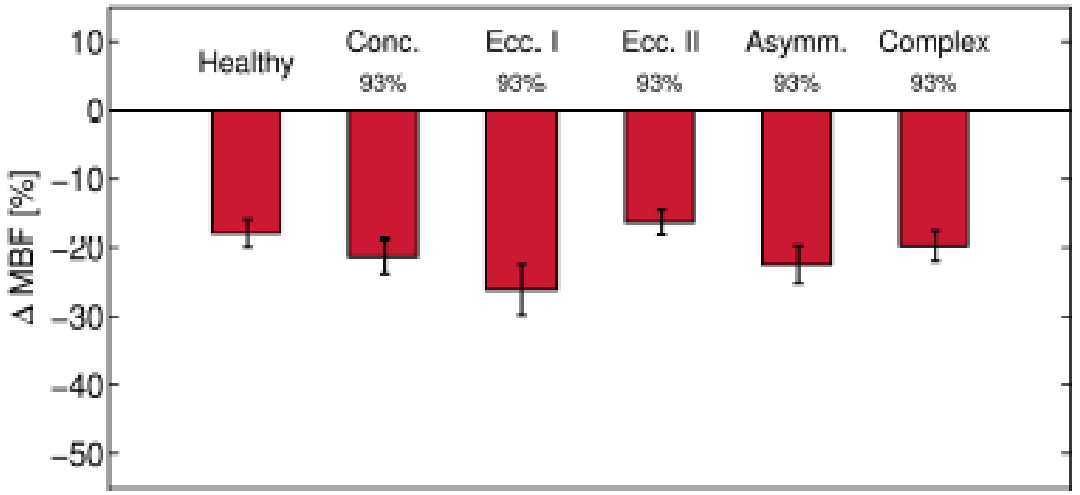


[4]

[4] K. Sommer et al., 2015.

Previous Results





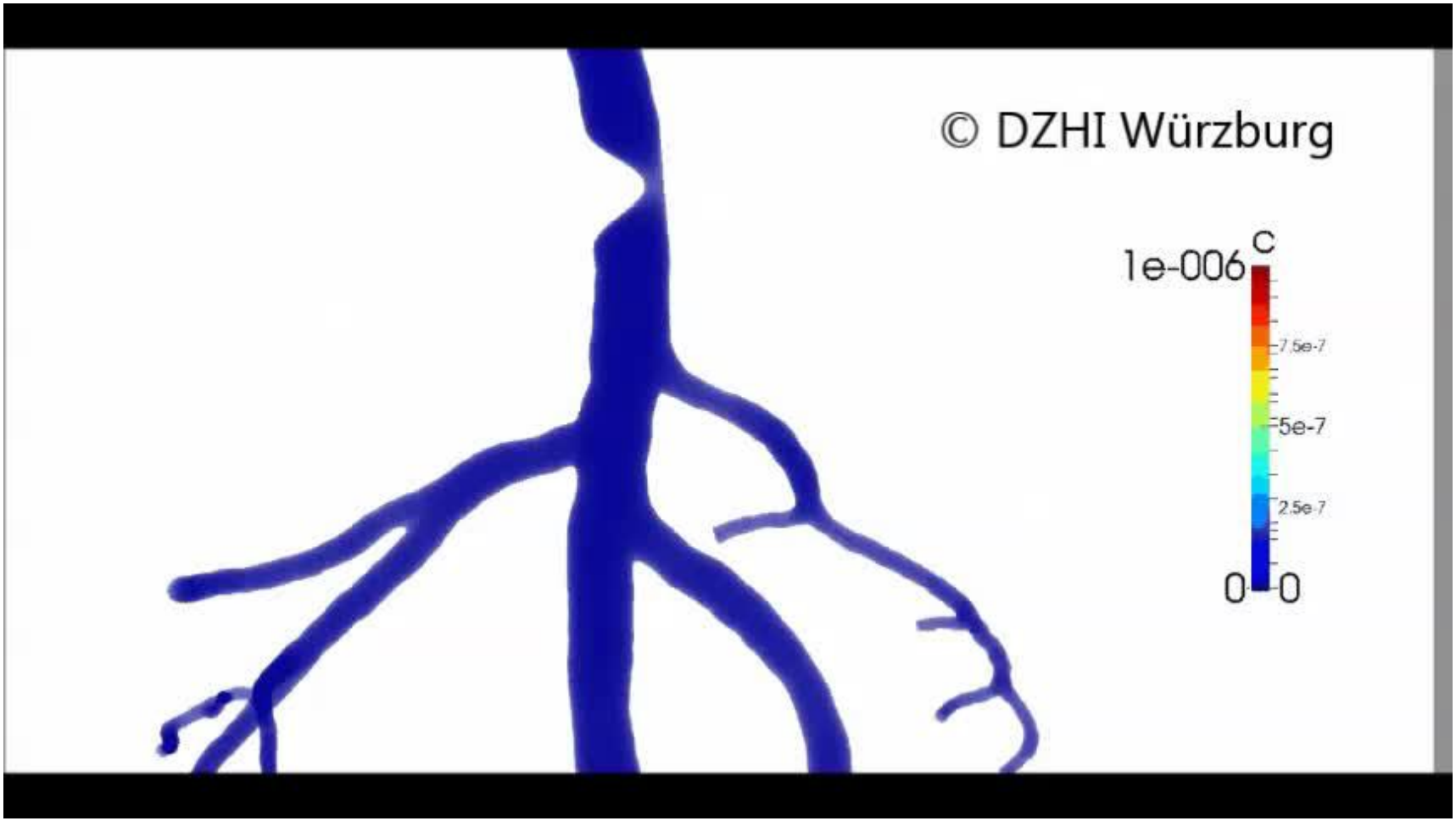
[4]

Complex dependencies on:
- Stenoses
- Branching angles
- Length and curvature of vessel sections

➡ Systematic errors, that cannot be neglected!

[4] K. Sommer et al., 2015.

Previous Results



[4]

Performed on cluster *elwetritsch* (University Kaiserslautern)

[4] K. Sommer et al., 2015.

Scalability Testing

Investigation of models in higher detail (>10 Mio cells)

⇨ Longer computation times

- Parallelization on larger systems

Problem:

#cores * T_{cycle} / writeInterval

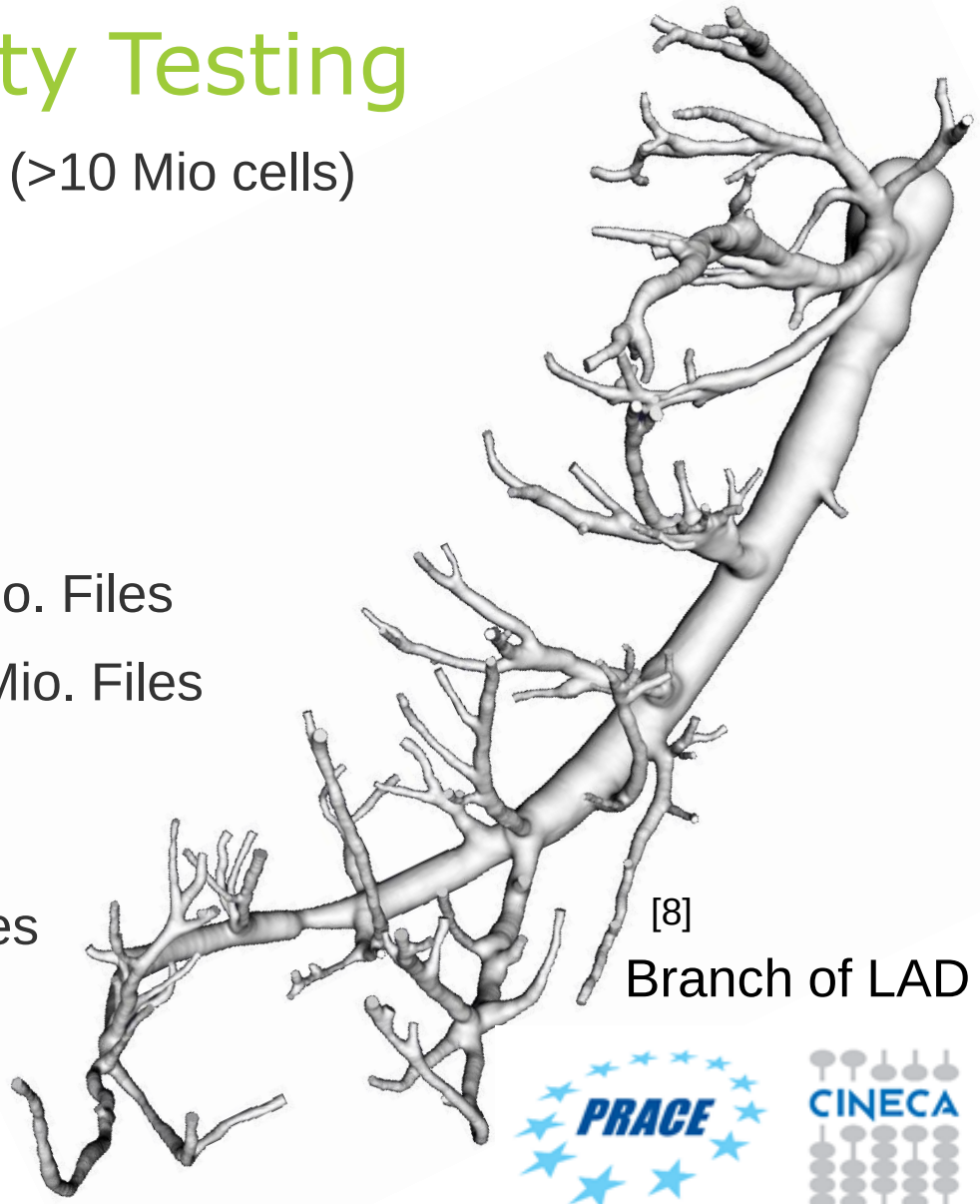
128 * 1s / 0.0001 s = ~12 Mio. Files

1024 * 1s / 0.0001 s = ~100 Mio. Files

⇨ Multiplication of I/O!

PRACE Prep Access:

- Computations on different model sizes (5 Mio cells vs 30 Mio cells)



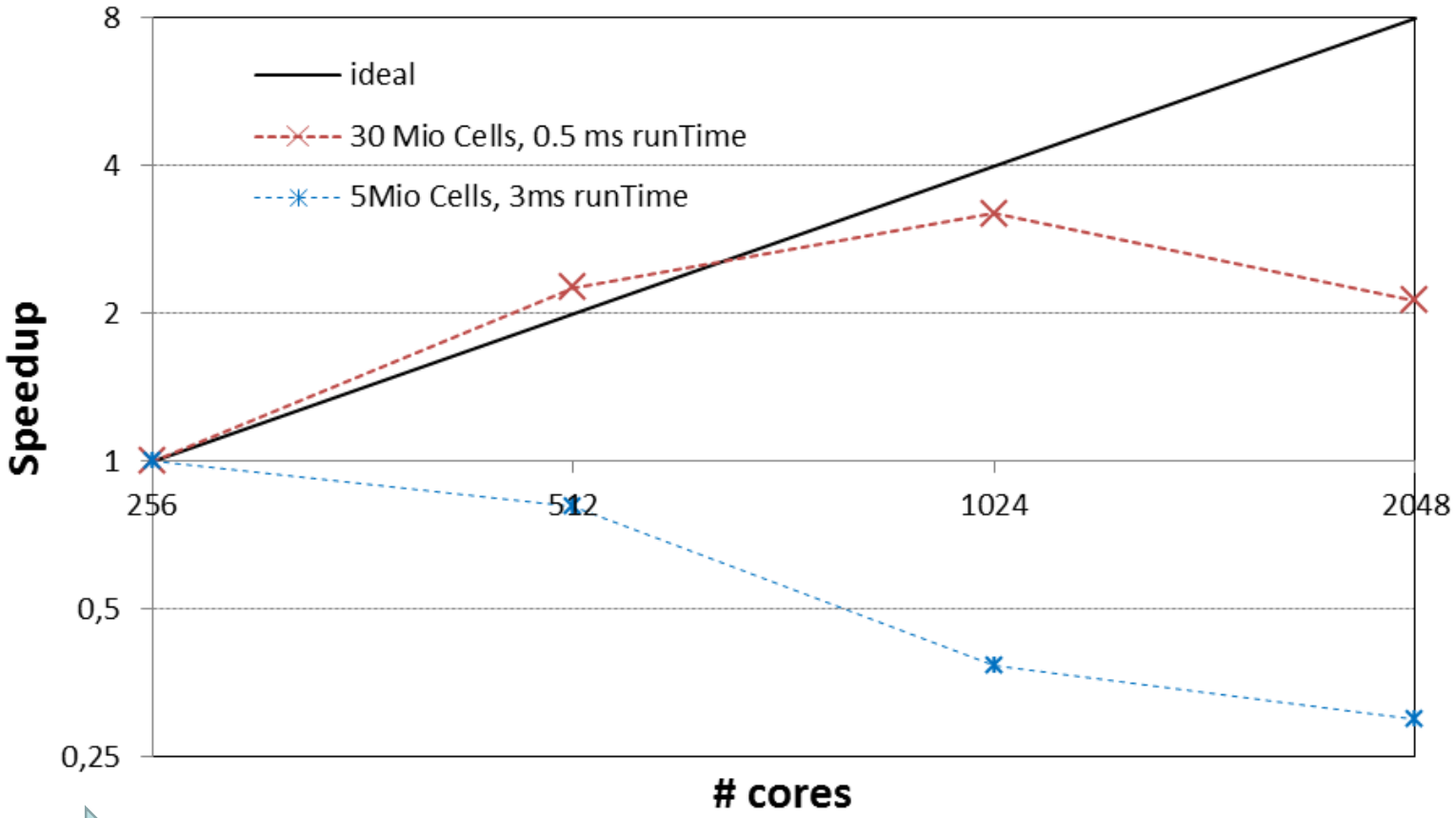
[8]

Branch of LAD

[8] CHFC, 2016.

Scalability Testing

Clocktime normalized to clocktime@256 cores



[8]

Improving performance on large grid sizes,
Prediction of «optimal configuration» for treated model

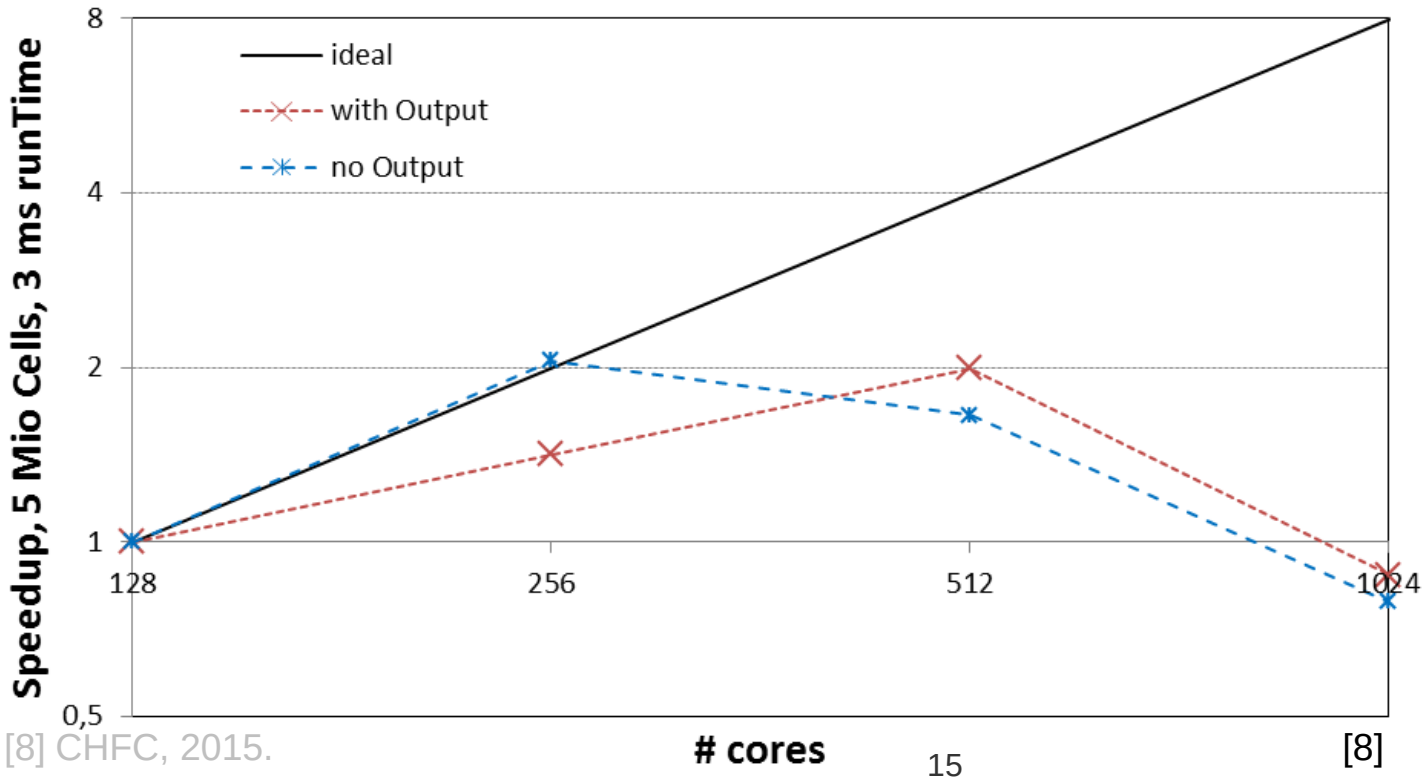
[8] CHFC, 2015.

Scalability Testing

- Comparison of clocktimes:
  - output vs no-output

	Clocktime [s] to simulated runTime 3 ms	
	with output	no output
128	980	869
256	692	423
512	492	525
1024	1117	1101

Clocktime normalized to clocktime@128 cores



[8] CHFC, 2015.

[8]

Conclusion

- Better performance on larger grid sizes
  - ➡ Utilization of HPC clusters justified

- Estimation of «perfect core number» for vascular models

Problems remain:

- Large output file numbers
- Many I/O operations
  - ➡ Need for file processing tool! (cooperation with HLRS)
- Time-consuming model creation and meshing process

Questions?

Thank You for Listening!

Thanks to:
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Prof. Dr. Maria Siebes, Biomedical Engineering & Physics, AMC Amsterdam

Chair for Cellular and Molecular Imaging
http://www.chfc.ukw.de/forschung/forschungsprofessuren/cmi.html

Bibliography

[1] Chareonthaitawee P. Kaufmann PA, Rimoldi O, Camici PG. Heterogeneity of resting and hyperemic myocardial blood flow in healthy humans. Cardiovasc Res 2001, 50:151-161.

[2] Jack Lee and Nicolas P Smith. The multi-scale modelling of coronary blood flow. *Annals of biomedical engineering*, 40(11):2399–413, 2012.

[3] Julia Hamer, Strömungsmechanische Untersuchungen zur kontrastmittelgestützten Magnetresonanztomographie der Herzdurchblutung, Diploma Thesis, 2009.

[4] Karsten Sommer, Simulation of Bolus Transport in Magnetic Resonance Perfusion Imaging using Realistic Vascular Geometries, Doctoral Thesis, 2015.

[5] MMID4 Manual, Version 2.3, 1998.

[6] http://www.vmtk.org/, Version 1.2, 2015.

[7] M. Siebes et al., Biomedical Engineering & Physics, AMC Amsterdam, 2014.

[8] CHFC (work in progress), 2015/6.