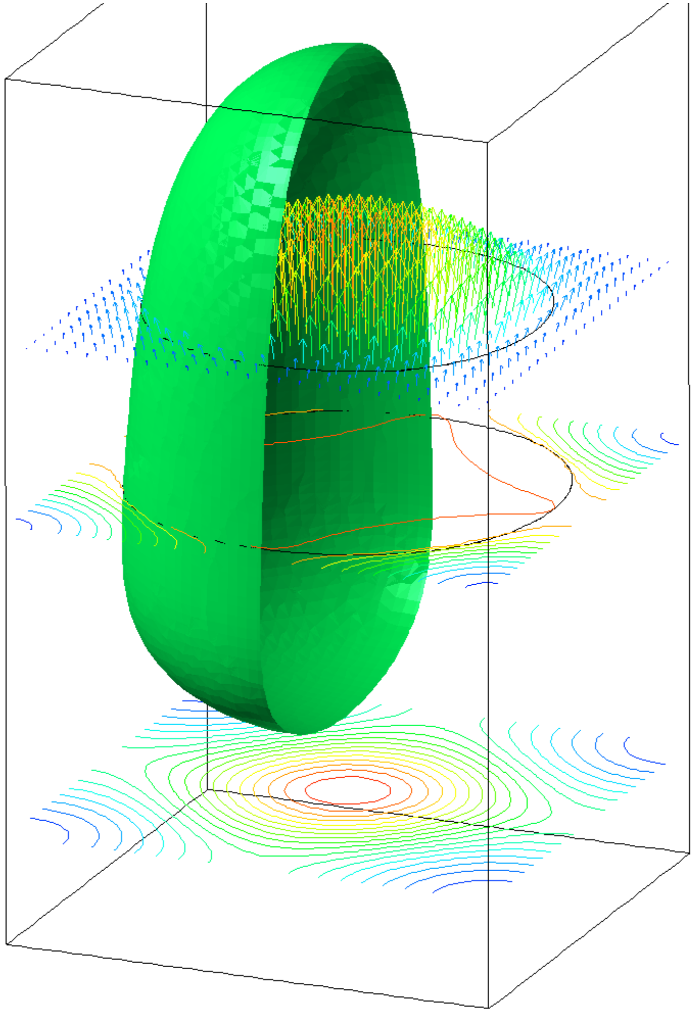
Karlsruher Institut für Technologie

Numerical investigations of gas-liquid flows in mini-channels for applications in chemical process engineering



Dr.-Ing. Martin Wörner

Institute for Nuclear and Energy Technologies
Chemical process engineering group

Workshop SimLab@KIT

Karlsruhe Institute of Technology
November 29-30, 2010

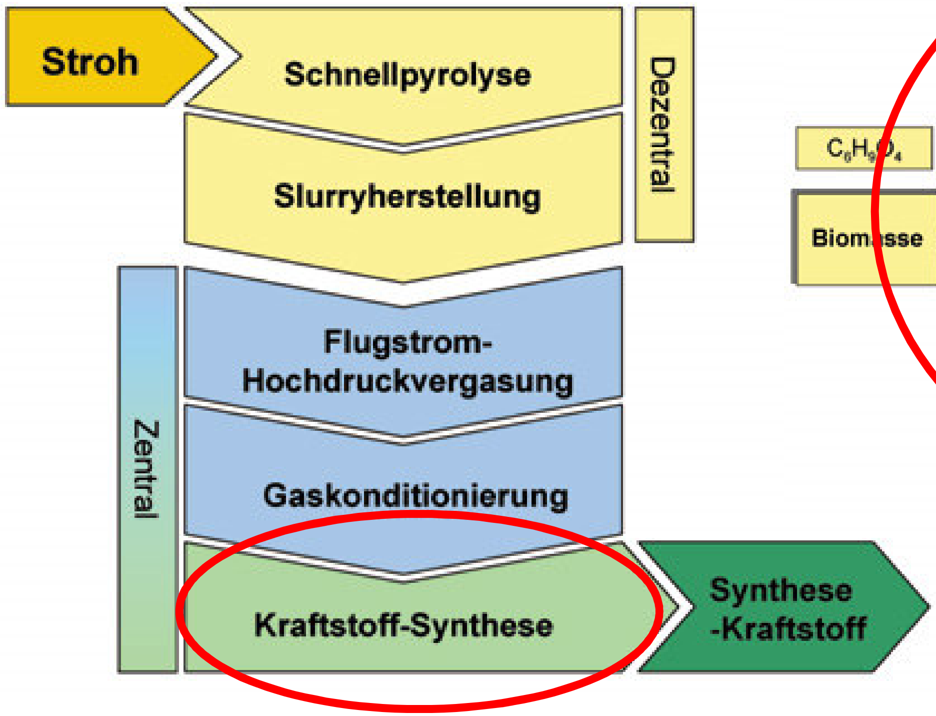
Outline

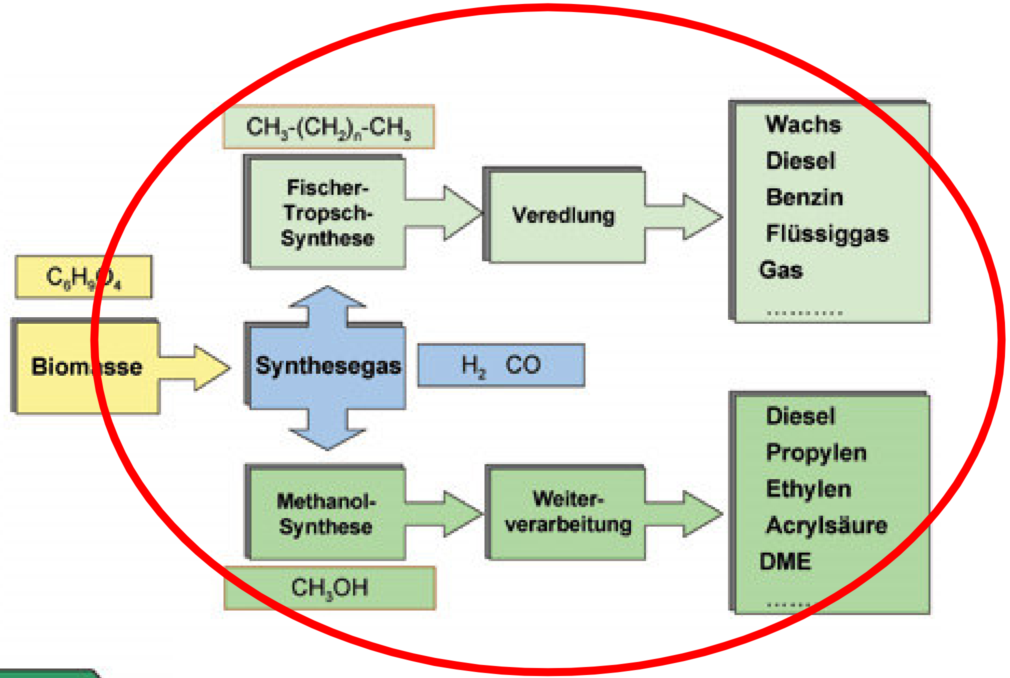
- Background and motivation
  - Technological: synthesis of biofuels
  - Scientific: Interaction between flow, transport and reaction
- Numerical simulation method
  - Governing equations and numerical method
  - Typical results for fluid flow and mass transfer
- Performance analysis of the code
  - NEC SX-8 and SX-9
  - hc3
- Conclusions

Technological background

- **Karlsruhe BTL (biomass-to-liquid) process** bioliq®

Process steps





Fuel synthesis:
a heterogeneously catalyzed gas-liquid process

http://iwrwww1.fzk.de/bioliq/index.html

Technological background

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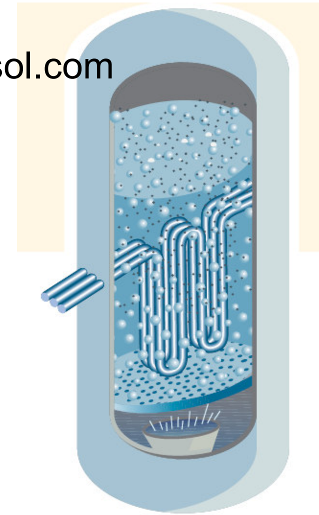
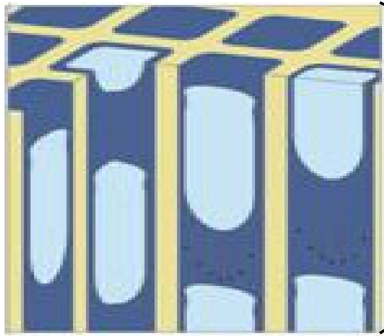
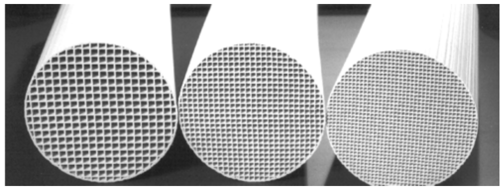
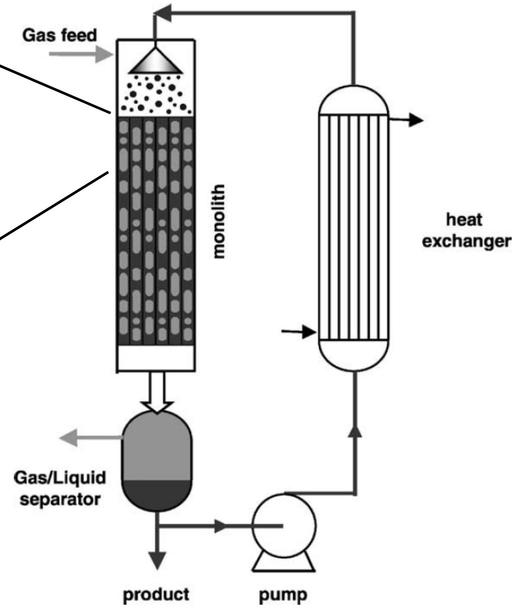
- Fischer-Tropsch-Synthesis (conversion of CO & H_2 into liquid fuels)
  - Sasol Inc: 6 Mio. t fuel per year by bubble column reactors (diam. 12 m)
  - Monolith reactors with Taylor flow offer higher yield by similar selectivity
    Güttel et al. Ind. Eng. Chem. Res. 47 (2008) 6589

www.sasol.com





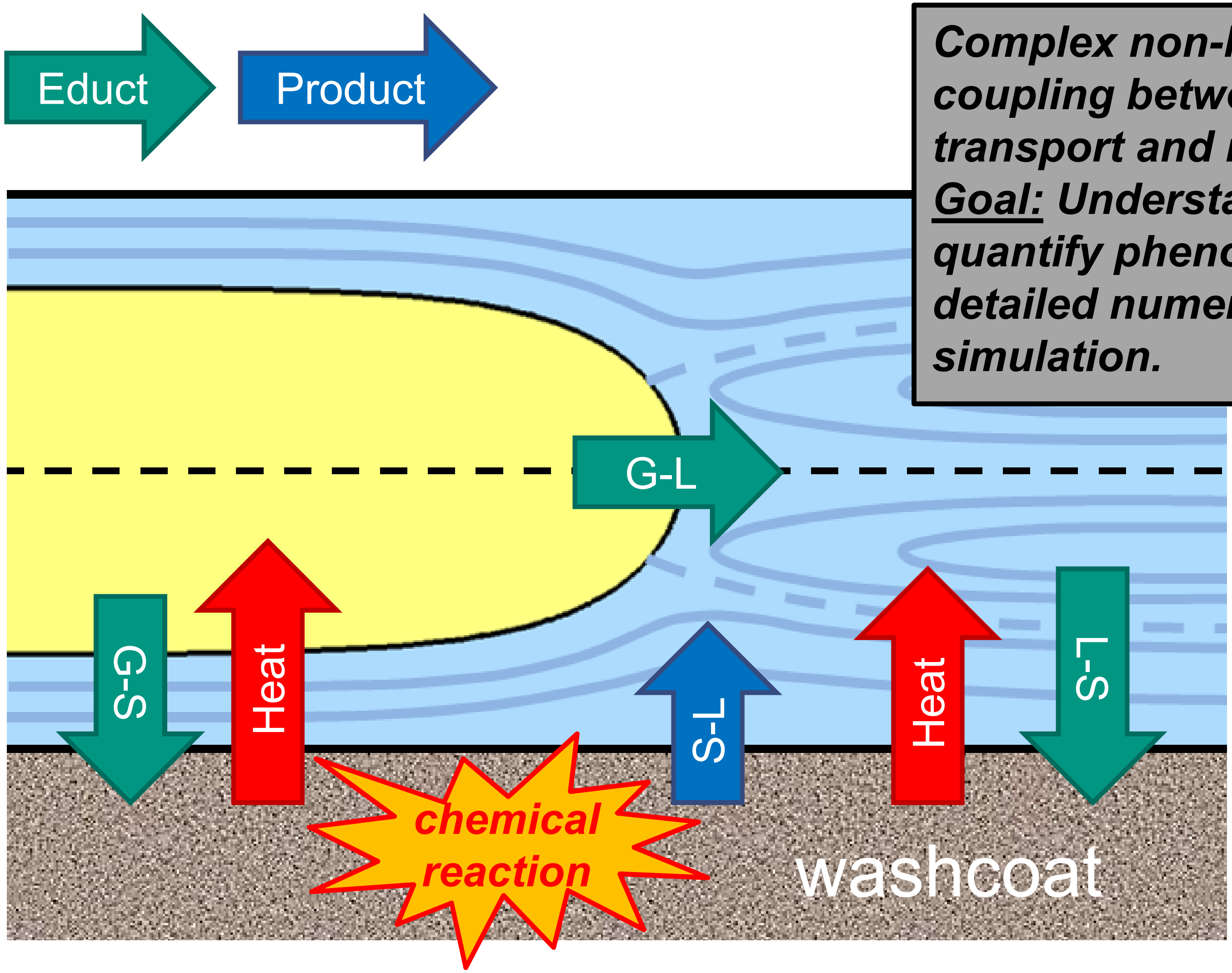




Monolith-Loop-Reaktor
de Deugd et al. Cat. Today 79 (2003) 495

- <u>Here:</u>
  - Investigate hydrodynamics of Taylor flow in a single square mini-channel by detailed numerical simulations

Scientific background



Complex non-linear coupling between flow, transport and reaction.
Goal: Understand and quantify phenomena by detailed numerical simulation.

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Governing equations

- Navier-Stokes equation in single field formulation with surface tension term for two incompressible immiscible Newtonian fluids with constant physical properties
- f = liquid volumetric fraction within a mesh cell $(0 \le f \le 1)$

$$\frac{\partial f}{\partial t} + \nabla \cdot f \mathbf{v}_{\mathrm{m}} = 0$$

$$\nabla \cdot \mathbf{v}_{\mathrm{m}} = 0$$

$$\rho_{\mathrm{m}} \equiv \frac{f \rho_1^* + (1-f)\rho_2^*}{\rho_1^*} \qquad \mu_{\mathrm{m}} \equiv \frac{f \mu_1^* + (1-f)\mu_2^*}{\mu_1^*}$$

$$\frac{\partial \rho_{\mathrm{m}} \mathbf{v}_{\mathrm{m}}}{\partial t} + \nabla \cdot \left(\rho_{\mathrm{m}} \mathbf{v}_{\mathrm{m}} \mathbf{v}_{\mathrm{m}}\right) = -\nabla P + \frac{\nabla \cdot \left[\mu_{\mathrm{m}} \left(\nabla \mathbf{v}_{\mathrm{m}} + \left(\nabla \mathbf{v}_{\mathrm{m}}\right)^{\mathrm{T}}\right)\right]}{Re_{\mathrm{ref}}} + \rho_{\mathrm{m}} Fr_{\mathrm{ref}} \hat{\mathbf{e}}_{\mathrm{g}} + \frac{Eu_{\mathrm{ref}}}{L_{\mathrm{axial}}} \hat{\mathbf{e}}_{\mathrm{axial}} + \frac{a_{\mathrm{i}} \kappa \hat{\mathbf{n}}_{\mathrm{i}}}{We_{\mathrm{ref}}}$$

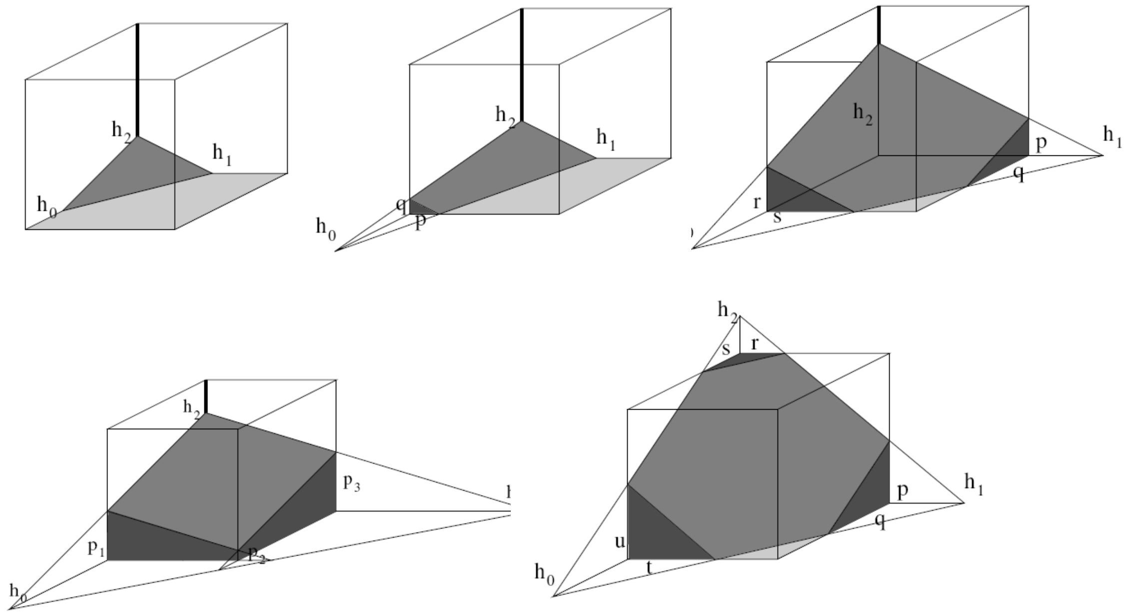
Numerical method*

- Finite volume discretization
- Structured 3D Cartesian grid (staggered)
  - equidistant in two directions, optionally non-equid. in third direction
- Approximation of spatial derivates by central differences
- Explicit 3rd order Runge-Kutta time integration scheme
- Projection method for pressure-velocity coupling
  - Resulting pressure Poisson equation is solved by LINSOL package developed at University Karlsruhe
- Volume-of-fluid method with interface reconstruction
- In-house computer code TURBIT-VOF
  - Fortran 77 and Fortran 90
  - The code is not parallelized yet

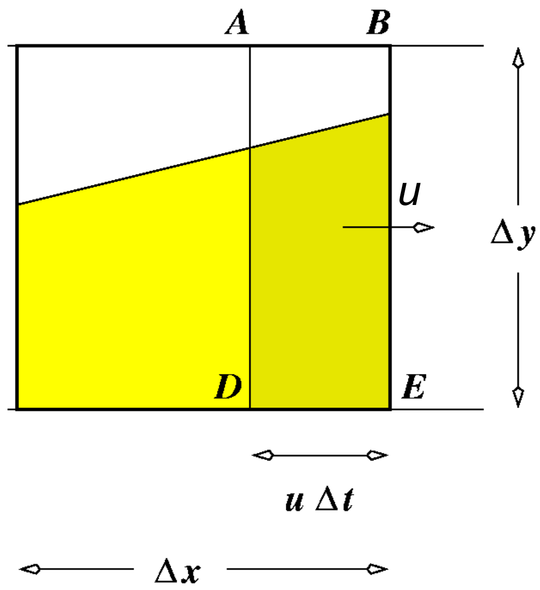
*see Öztaskin et al. Phys. Fluids **21** (2009) 042108

Interface reconstruction

- In each mesh with both phases (i.e. where $0 < f < 1$) the interface is locally approximated by a plane
- The location and orientation of this plane is reconstructed from the distribution of f in neighboring mesh cells



Flux computation



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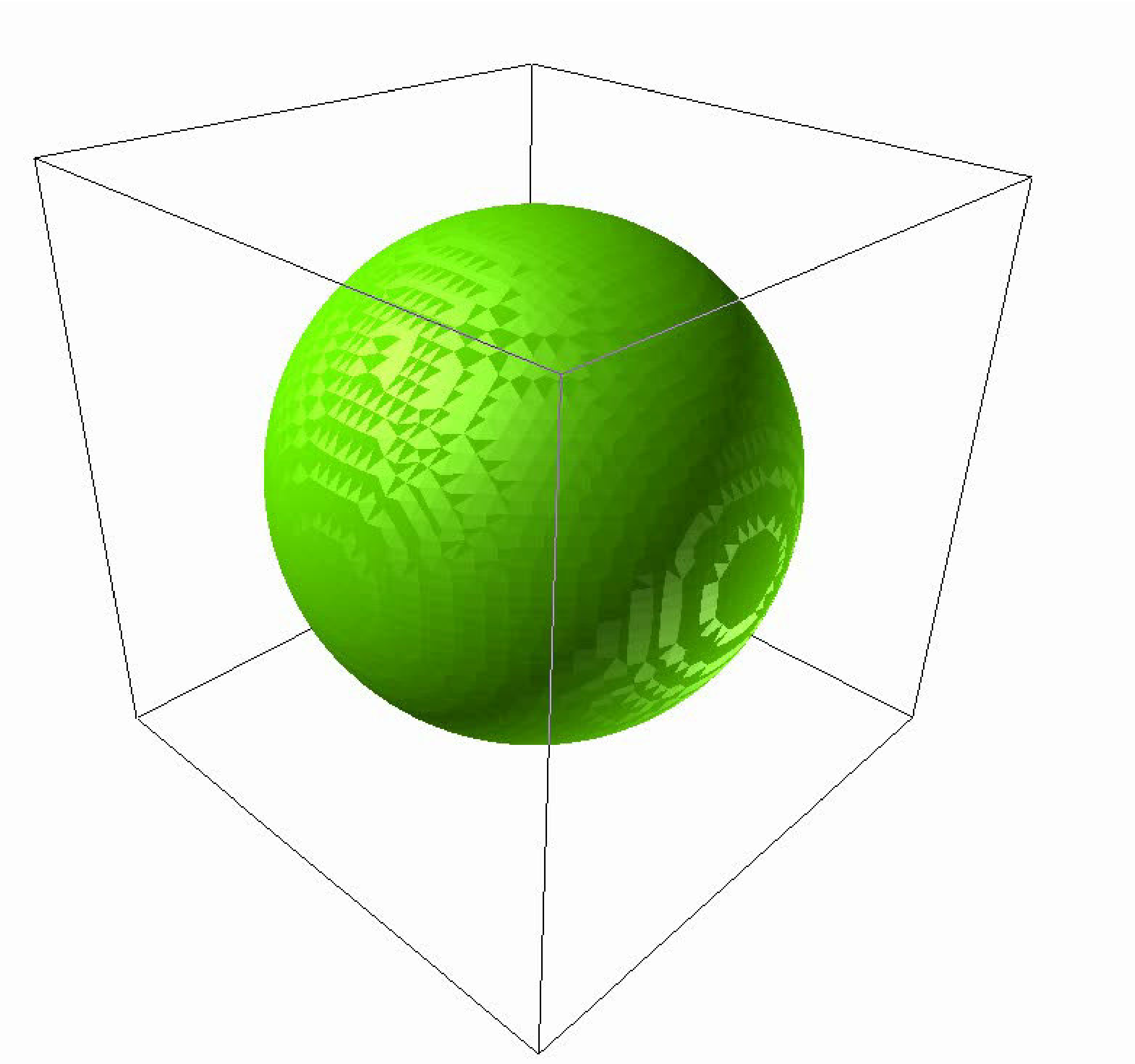
Simulation results



Computed bubble shapes

$1\,\text{mm} \times 1\,\text{mm}$

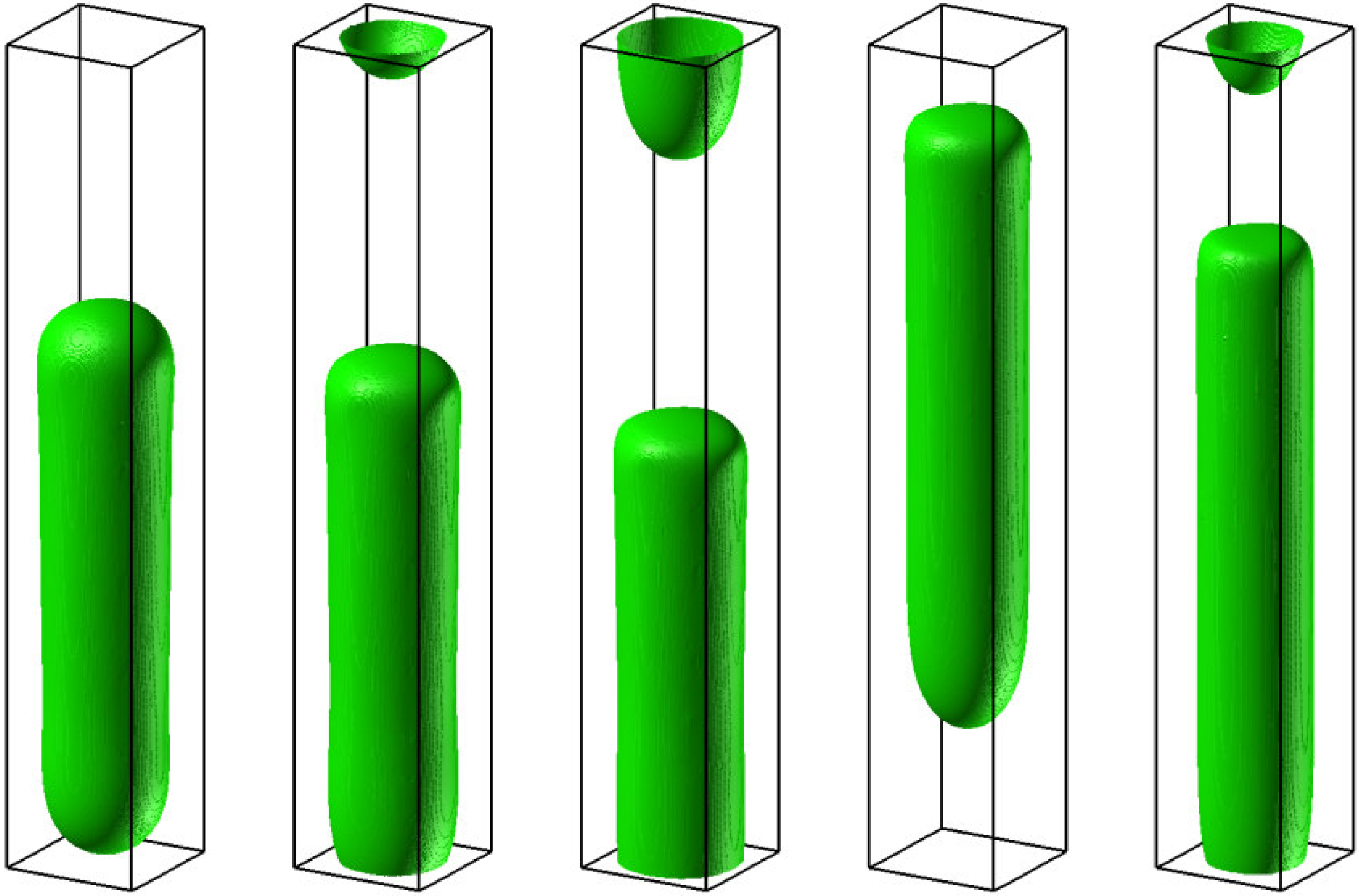
$L_{uc} = 6\,\text{mm}$

$\varepsilon_G = 0.4$

$$\frac{Re}{Ca} = \frac{\sigma \rho_L D_h}{\mu_L^2} \equiv La = 27.27$$

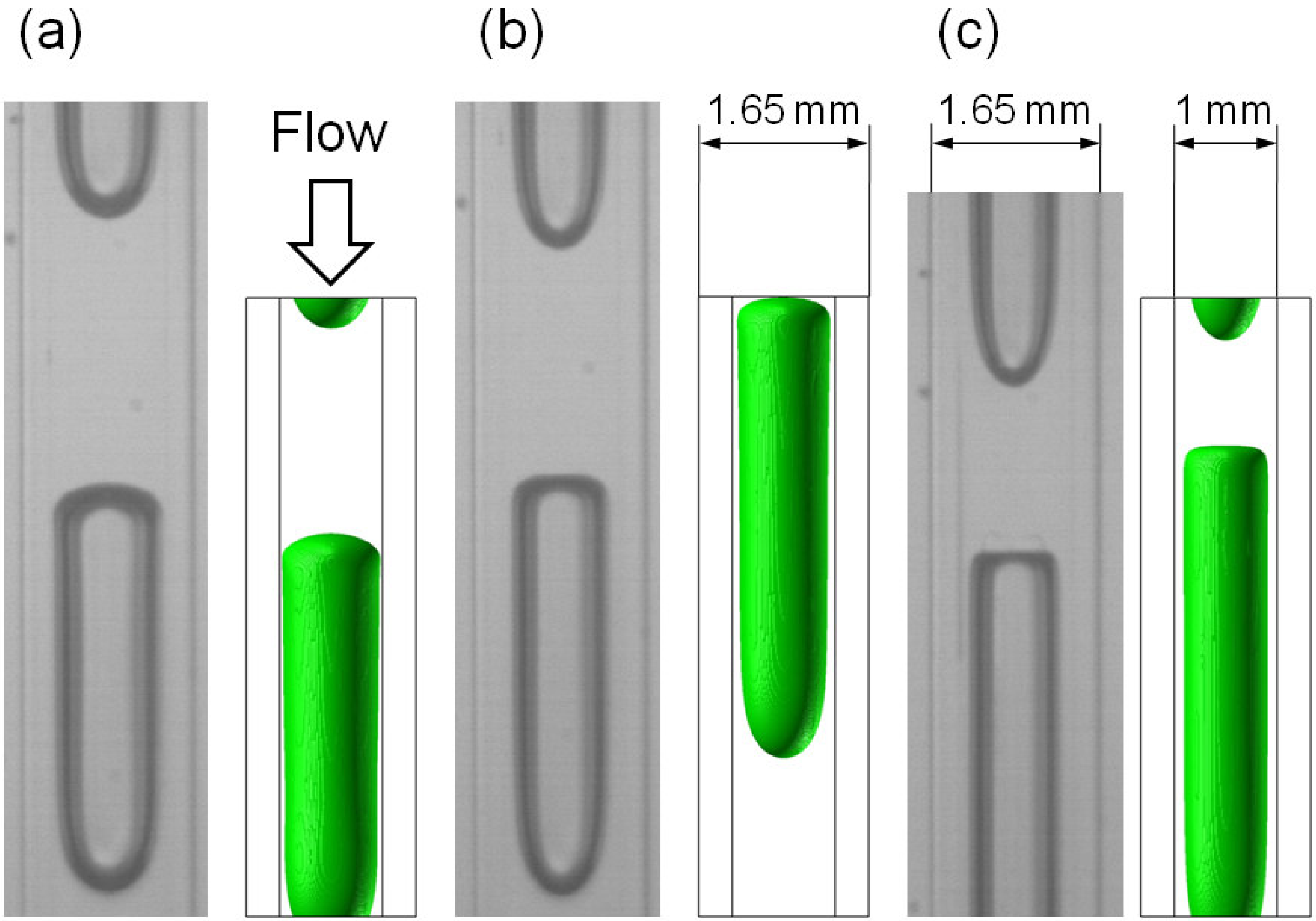
$$Ca \equiv \frac{\mu_L U_B}{\sigma}$$

$$Re \equiv \frac{\rho_L D_h U_B}{\mu_L}$$



Ca =	0.045	0.12	0.17	0.26	0.49
Re =	1.22	3.19	4.64	7.16	13.4

Experimental validation*



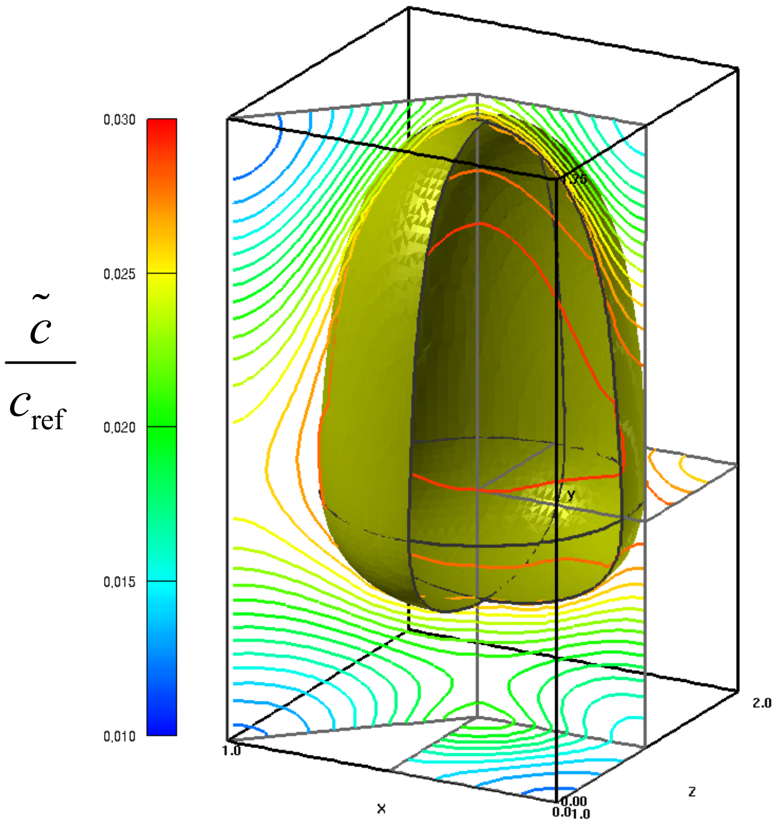
Keskin et al. AIChE J. **56** (2010) 1693–1702

** Experiments by T. Bauer and R. Lange*

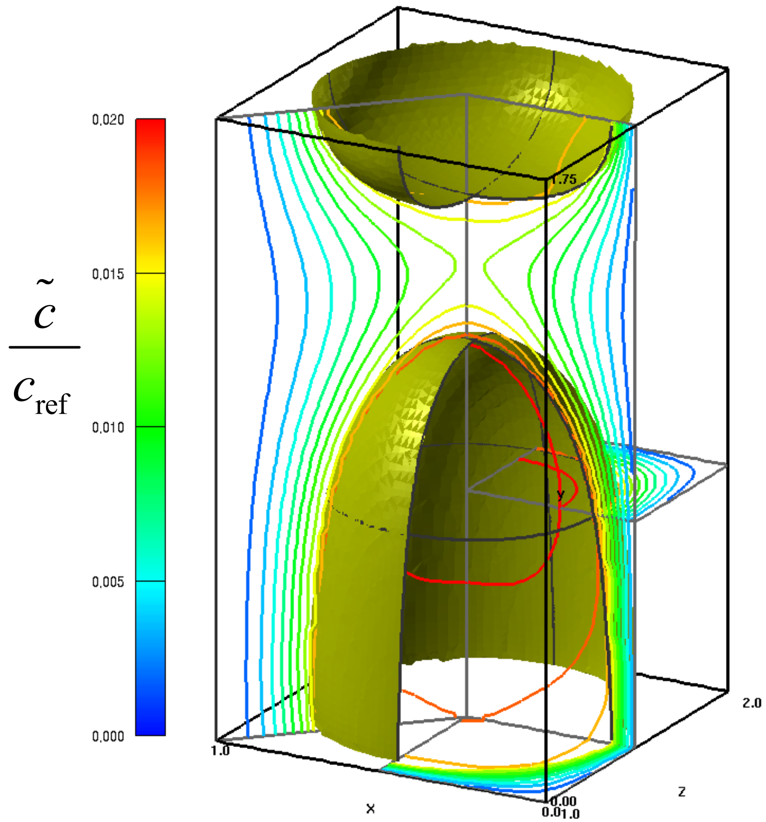
TECHNISCHE UNIVERSITÄT DRESDEN

Mass transfer and chemical reaction

- Without chemical reaction
- <u>Fast</u> heterog. reaction (1st o.)



short bubbles are more efficient



long bubbles are more efficient

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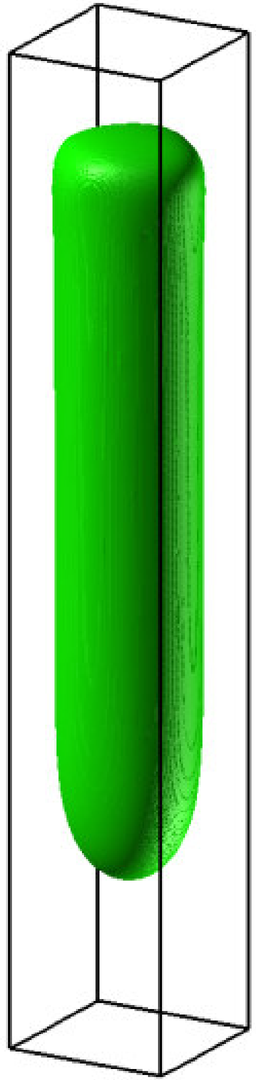
Test case for benchmarking

- Grid 80×480×80 mesh cells (about 3 million in total)
- Computation of 10 time steps
- Hardware
  - NEC SX-8 (sxf90 compiler)
  - NEC SX-9
  - hc3 (Intel compiler)
  - All runs on a single processor
  - Memory requirement 4GB



NEC SX-8: F_PROGINF=DETAIL

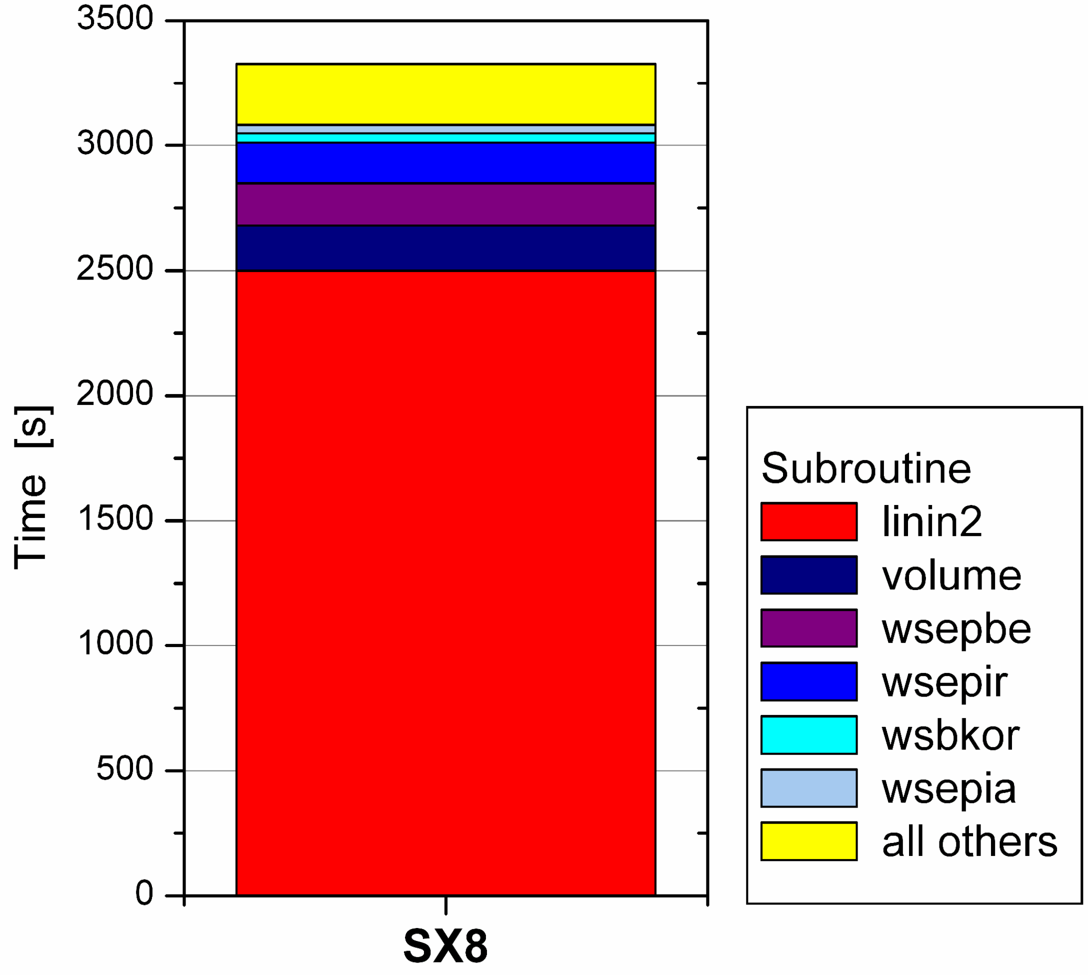
```
******  Program Information  ******
 Real Time (sec)         :        35032.602790
 User Time (sec)         :        33705.743498
 Sys  Time (sec)         :          143.167463
 Vector Time (sec)       :        29690.202492
 Inst. Count             :       597647716096 8.
 V. Inst. Count          :       1471193564599.
 V. Element Count        :     370048534017314.
 FLOP Count              :     134402975301641.
 MOPS                    :        11112.462706
 MFLOPS                  :         3987.539255
 VLEN                    :          251.529468
 V. Op. Ratio (%)        :           98.797160
 Memory Size (MB)        :         4032.031250
 MIPS                    :          177.313316
 I-Cache (sec)           :           94.098275
 O-Cache (sec)           :          731.221560
 Bank (sec)              :         2824.320016
```

(100 time steps)

Flow trace analysis for SX-8

PROG.UNIT	FREQUENCY	EXCLUSIVE TIME[sec](%)	AVER.TIME [msec]	MOPS	MFLOPS	V.OP RATIO	AVER. V.LEN	VECTOR TIME
linin2	10	2499.715(75.1)	249971.500	13672.0	4921.2	99.37	256.0	2499.365
volume	13165932	181.144(5.4)	0.014	647.0	111.1	47.16	24.2	49.248
wsepbe	103814562	168.516(5.1)	0.002	282.9	8.0	0.00	0.0	0.000
wsepir	415258248	160.700(4.8)	0.000	308.5	158.4	0.00	0.0	0.000
wsbkor	10802207	39.003(1.2)	0.004	275.4	42.2	0.00	0.0	0.000
wsepia	1590	34.446(1.0)	21.664	280.4	25.3	0.00	0.0	0.000
putfb3	1	30.856(0.9)	30856.229	439.9	18.7	2.81	256.0	0.056
getfb3	1	28.885(0.9)	28885.197	488.7	6.9	0.00	28.1	0.000
fvn	2229034	17.924(0.5)	0.008	209.7	15.2	0.00	0.0	0.000
wsepic	31136532	14.283(0.4)	0.000	397.0	154.0	0.00	0.0	0.000
wsepbc	7784133	13.074(0.4)	0.002	241.7	6.0	0.00	0.0	0.000
wssta1	880	12.569(0.4)	14.282	563.6	76.9	0.00	0.0	0.000
bterm	1010916	9.707(0.3)	0.010	243.4	23.1	0.68	8.0	0.165
ofsber	2043501	9.618(0.3)	0.005	232.1	23.2	0.00	21.2	0.000
nvtouv	24522012	9.206(0.3)	0.000	149.8	49.3	0.00	0.0	0.000
wslins	10	9.031(0.3)	903.084	923.3	186.2	9.55	152.5	0.087
wsreko	880	8.714(0.3)	9.902	527.8	24.4	0.00	0.0	0.000
envber	1112019	7.473(0.2)	0.007	322.1	20.4	0.05	34.5	0.002
area	3032748	7.295(0.2)	0.002	581.8	116.2	57.95	23.9	2.350
wseb1	7784133	6.681(0.2)	0.001	203.2	29.1	0.00	0.0	0.000
gbpgc	10	6.488(0.2)	648.821	373.3	24.7	19.73	48.5	0.640
wsfvkx	2400	6.420(0.2)	2.675	382.0	20.0	0.03	36.2	0.001

Flow trace analysis for SX-8



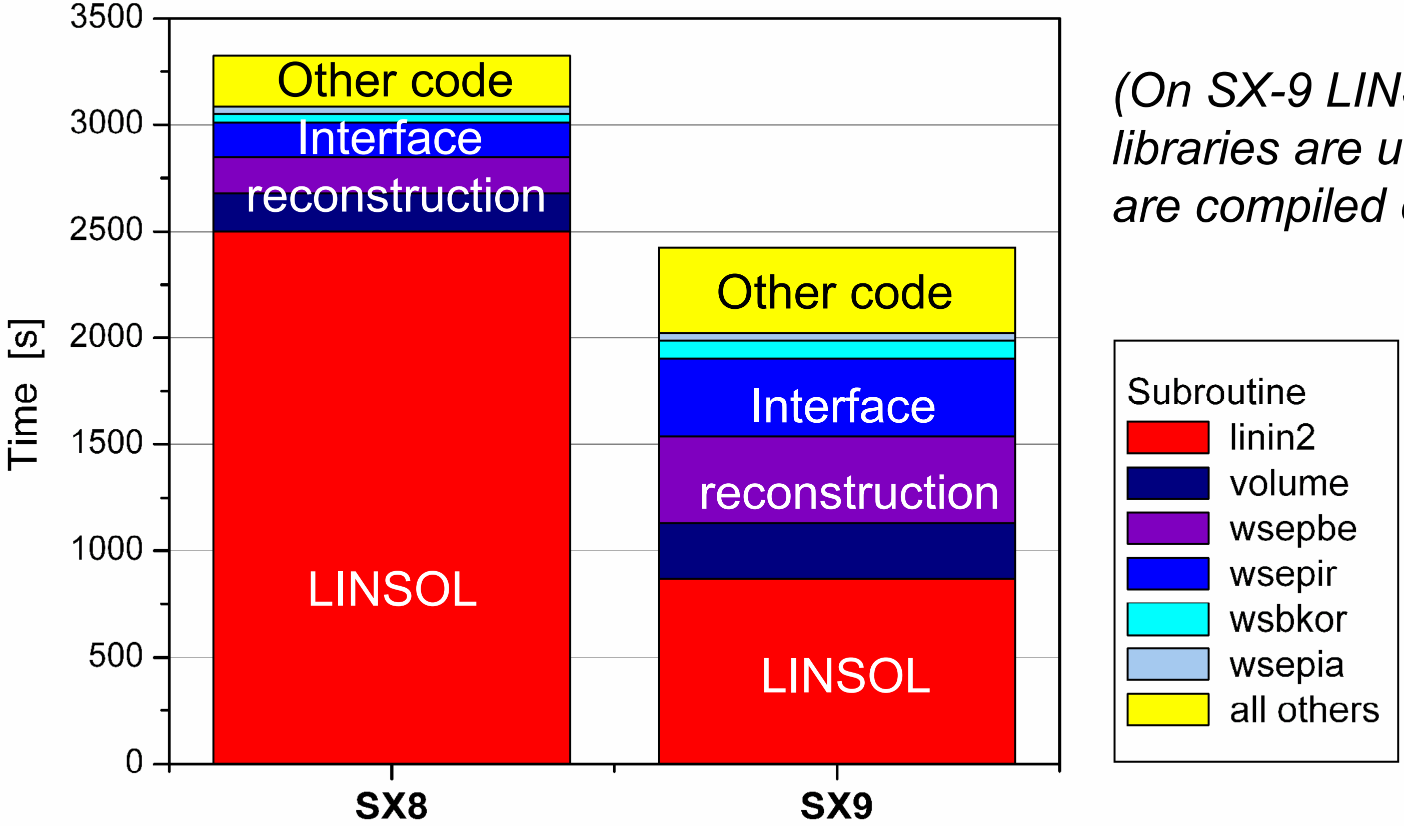
V.OP
RATIO

99.37 ***Poisson solver***

47.16
0.00
0.00
0.00
0.00

Interface reconstruction

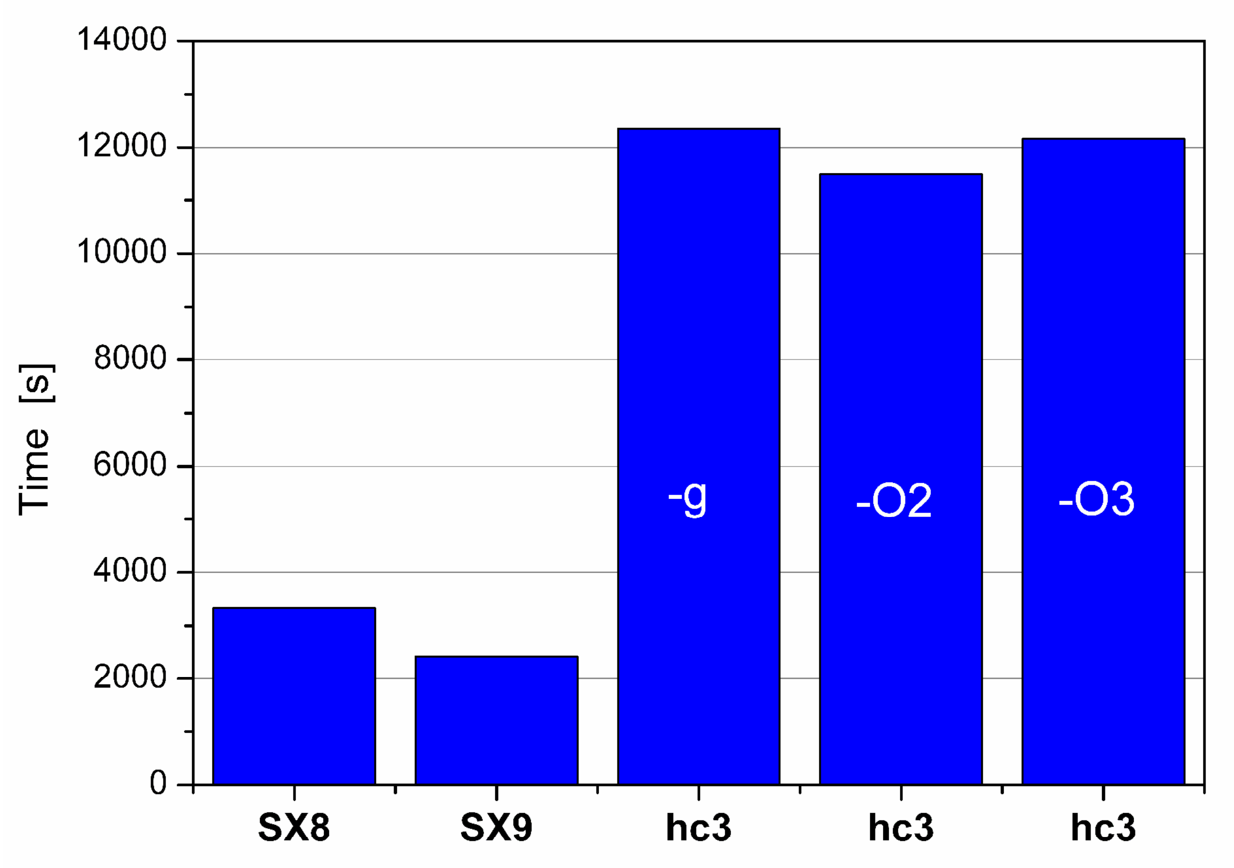
Comparison NEC SX-8 and SX-9



(On SX-9 LINSOL libraries are used which are compiled on SX-8)

- CPU time on SX-9 is about 27% lower than on SX-8
- Vector code (LINSOL) is on SX-9 about 65% faster than on SX-8
- Scalar code (IR) is on SX-9 more than 100% slower than on SX-8

Comparison SX-8/SX-9 and hc3



- CPU time on hc3 is more than three times larger than on SX-8
- On hc3 optimization options have a minor effect because about 97% of the total CPU time is used by LINSOL library which is already optimized

Conclusions

- Strategies for optimization of TURBIT-VOF code
  - Usage of LINSOL (suggestions by H. Häfner)
    - Test performance of different CG solvers available within the LINSOL package
    - Test weaker residuum criterion (currently 10^{-8})
  - NEC SX-8 and SX-9
    - Try to vectorize critical interface reconstruction subroutines
  - hc3
    - Run unparallelized TURBIT-VOF code on a single processor but branch to multiple processors when LINSOL is called (parallelized version of LINSOL is available)

Acknowledgement

- Many thanks to SimLab Energy especially to Daniela Piccioni-Koch and Hartmut Häfner