Experimental Verification of the Parallel Free Surface Lattice Boltzmann Method in waLBerla

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Chair for Computer Science 10 – System Simulation

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Motivation

Motivation


HydroGen4
BRENNSTOFFZELLE
NULL EMISSIONEN
GG HY 411


HydroGen4
BRENNSTOFFZELLE
NULL EMISSIONEN

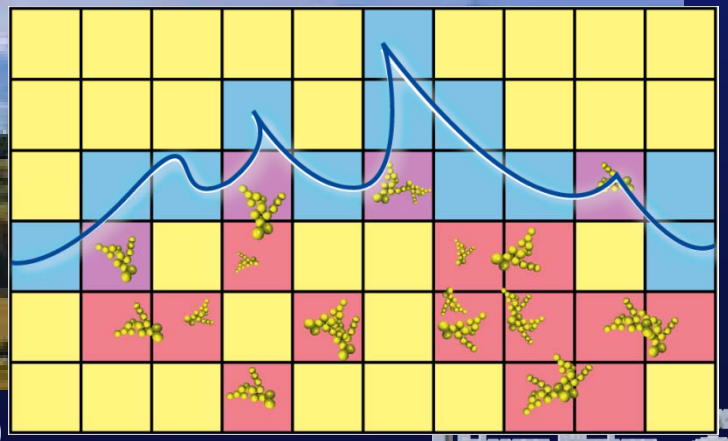
Outline

- waLBerla: A Large-Scale Lattice-Boltzmann Solver
- Free Surface Lattice Boltzmann
  - Lattice Boltzmann method
  - Free surface extension
  - Large-scale applications
- Validation
  - Possible parameter space
  - Experimental setup
  - Results

waLBerla

Widely applicable lattice Boltzmann from Erlangen

- CFD project based on lattice Boltzmann method
- Modular software concept
  - Supports various applications, currently planned:
    - Blood flow in aneurysms
    - Moving particles and agglomerates
    - Free surfaces to simulate foams, fuel cells, a.m.m.
    - Charged colloids
    - Brownian Motion
  - Integration in efficient massive-parallel environment

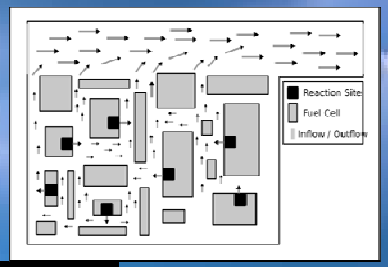


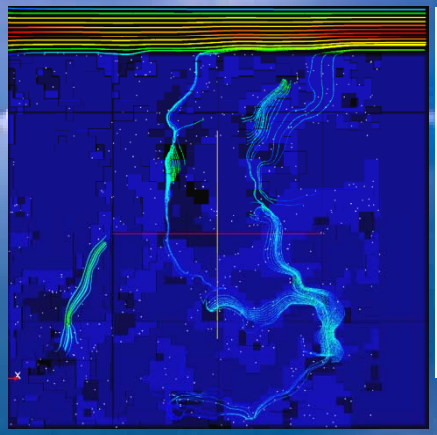
- Patch concept enables
  - Mixture of applications
  - Parallelization
  - Load Balancing

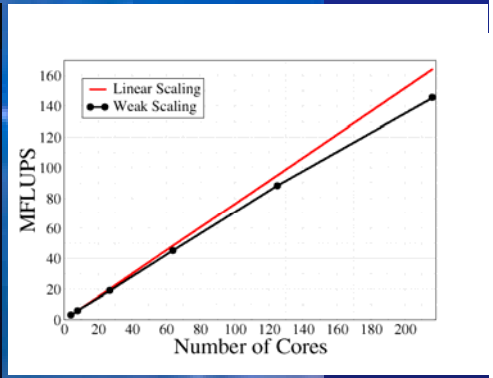
waLBerla

Widely applicable lattice Boltzmann from Erlangen

- Homogeneous Mixture Flows
  - Simulation of solid oxide fuel cells

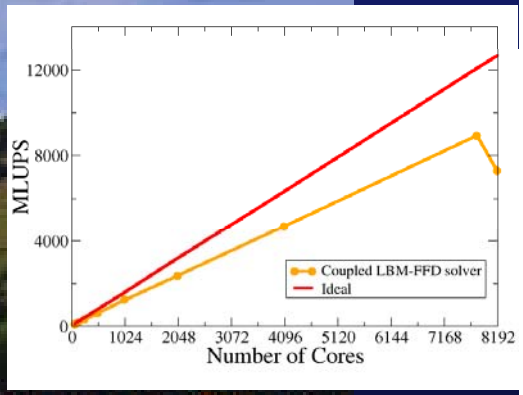






Video

- Large-Scale Particulate Flows
  - Largest Simulation:
    - 264 million particles
    - $1.5 \cdot 10^{11}$ lattice cells



Simulation of many particles in $1.3 \cdot 10^8$ lattice cells

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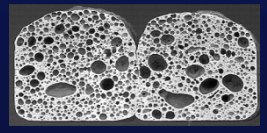
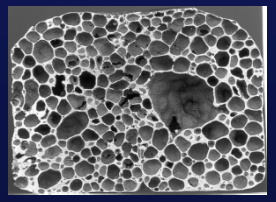
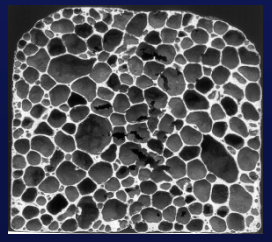
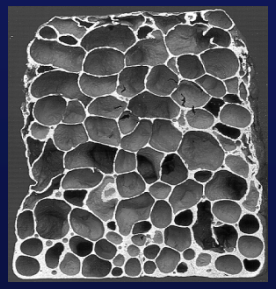
Free Surface: Simulating Metal Foams

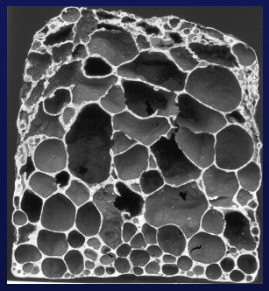
Collaboration with
Dept. of Material Sciences
Prof. Singer, Dr. Körner

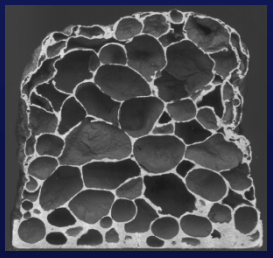












Lattice Boltzmann Method

- Boltzmann Equation

$$\partial_t f + F \cdot \partial_p f + \xi \cdot \nabla f = \Omega$$

ξ ... particle velocity
F ... external forces
Ω ... collision operator

- Simplest Collision Model: BGK

$$\partial_t f + \xi \cdot \nabla f = -\frac{1}{\lambda}[f - f^{(0)}]$$

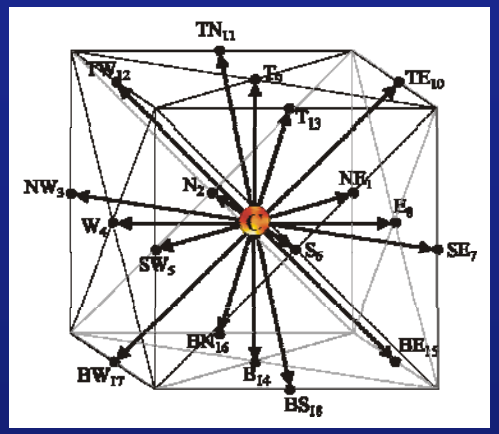
ξ ... particle velocity
$f^{(0)}$ ... equilibrium distribution function
λ ... relaxation time

- Macroscopic Quantities

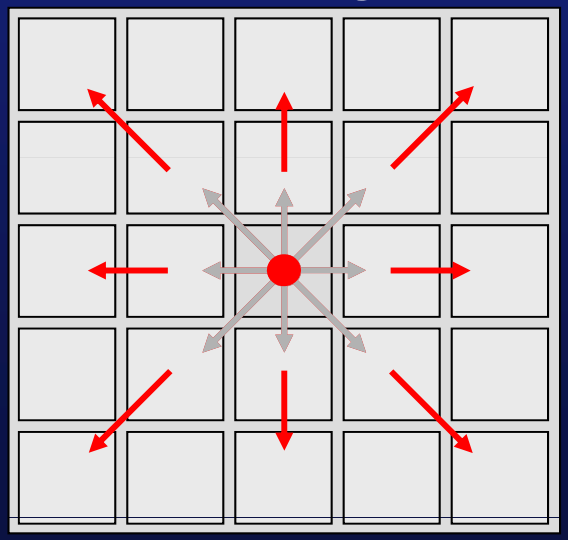
$$\rho = \sum_\alpha f_\alpha \qquad \rho u = \sum_\alpha e_\alpha f_\alpha$$

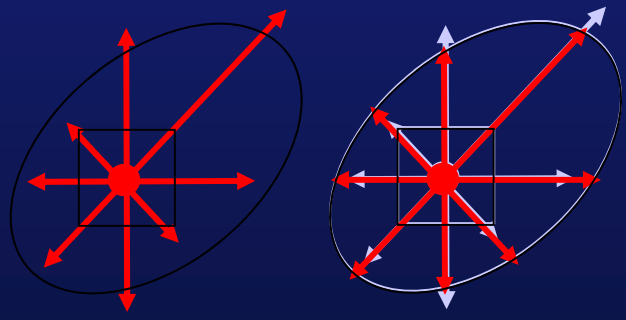
Lattice Boltzmann Method

- Discretization



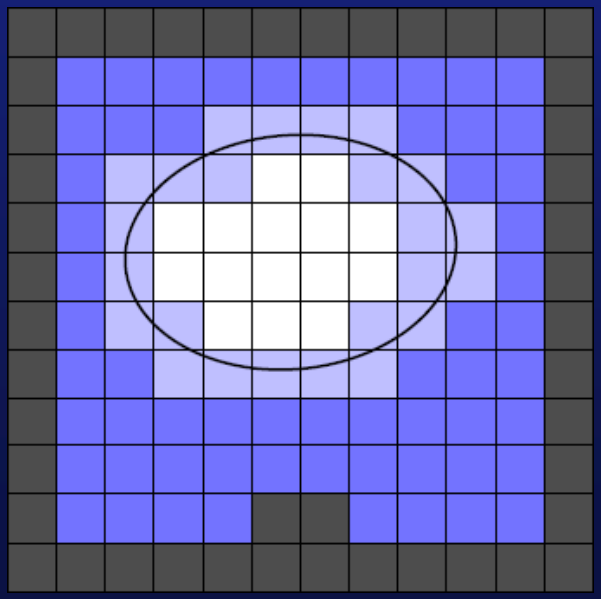
- Streaming and Relaxation

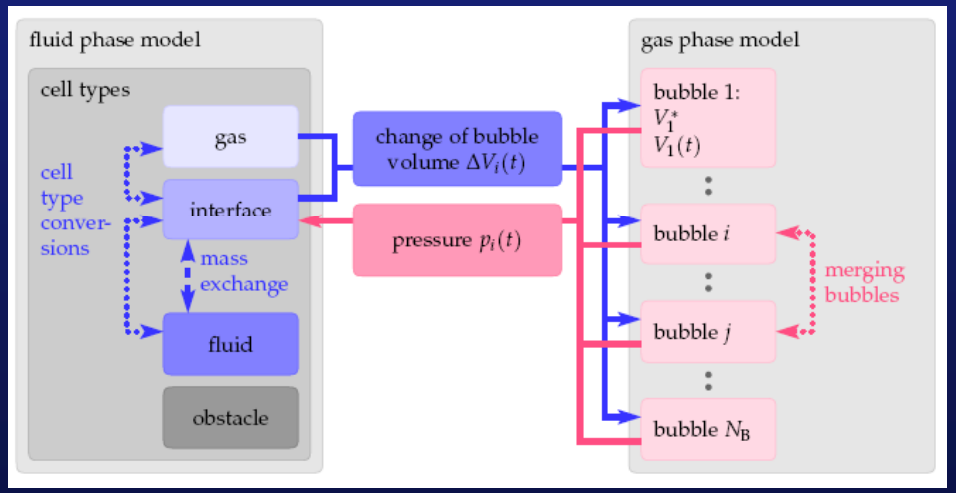




Free Surface-LBM

- „Free surface“ is „two phase“, however:
  - Compute only liquid phase
  - Model gas phase by ideal gas equation (no flow but only pressure is modeled)



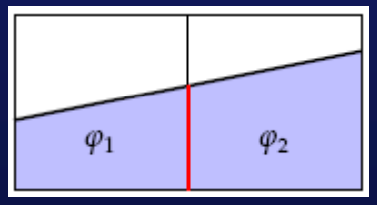


Free-Surface LBM
Fraction of fluid volume in Interface cells

- Interface cells store fluid fraction (similar to VoF)
- Fluid advection:
  - Mass transfer between interface and liquid cells
  - Mass is conserved

$$\Delta m_i(x,t) = \begin{cases} 0 & \text{for} \quad (x+c_i) \in \mathcal{C}^{\mathrm{G}} \\ F_{\mathrm{T}}(x+c_i,t) - F_i(x,t) & \text{for} \quad (x+c_i) \in \mathcal{C}^{\mathrm{F}} \\ \frac{1}{2}\left[\varphi(x,t) + \varphi(x+c_i,t)\right]\left[F_{\mathrm{T}}(x+c_i,t) - F_i(x,t)\right] & \text{for} \quad (x+c_i) \in \mathcal{C}^{\mathrm{I}} \end{cases}$$

  - For two interface cells a weighting factor depends on the fill levels



Free-Surface LBM
Interface boundary condition

- Simplification of stress tensor at interface
  - Navier-Stokes for incompressible fluid

$$\rho\delta_t\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} = \nabla\sigma$$

  - with stress tensor

$$\sigma_{ik} = -p_G(\vec{x},t)\delta_{ik} + \rho\nu(\delta_k u_i(\vec{x},t) + \delta_i u_k(\vec{x},t))$$

  - Treating gas as inert phase with vanishing density reduces stress to sole influence of pressure

$$p_G = p_V + p_\gamma$$

Free-Surface LBM
Interface boundary condition: gas pressure

- Gas volume pressure
  - Initial state with initial gas volume
  - Tracking gas volume changes in all interface cells leads to current volume
  - Pressure is ratio of current volume to initial volume

$$p_V = \frac{V^{init}}{V(t)}$$

  - Remarks:
    - Tracking gas volume changes throughout a parallel simulation involves means of all-to-all communication
    - Gas pressure depends on accurate mass tracking in interface cells
    - Supports continuous inflation of bubbles

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Free-Surface LBM
Interface boundary condition: surface tension

- Surface tension
  - Energy balance relates pressure to surface tension:

$$p_\gamma \cdot dV = \gamma \cdot dA$$

  - Young-Laplace equation (for 3 dimensions)

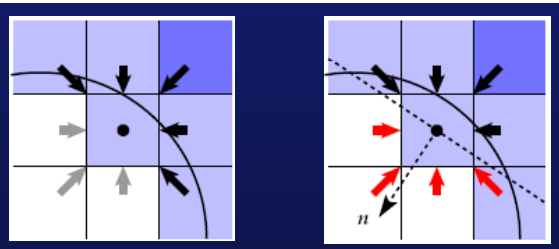
$$p_\gamma = 2\gamma\kappa(\vec{x}, t)$$

  - Takes only mean curvature into account, which is the mean value of the two principal curvatures

Free-Surface LBM
Interface boundary condition in LBM

- Reconstruction of distribution functions at interface
  - Simplified stress tensor means in LBM:
    - Velocity of fluid and gas phase have to be equal at interface
    - Force of the gas has to be balanced with force by fluid
  - Reconstruct distribution functions pointing in opposite direction of surface normal

$$F_i'(x-c_i,t) = F_i^0(\rho_G, v) + F_{\bar{i}}^0(\rho_G, v) - F_{\bar{i}}'(x,t) \quad , \quad x \in \mathcal{C}^{\mathrm{I}} \wedge \left[(x-c_i) \in \mathcal{C}^{\mathrm{G}} \vee c_i \cdot n(x,t) < 0\right]$$



  - Density of gas phase is computed from gas pressure

$$\rho_G = \frac{1}{c_s^2} \cdot p_G$$

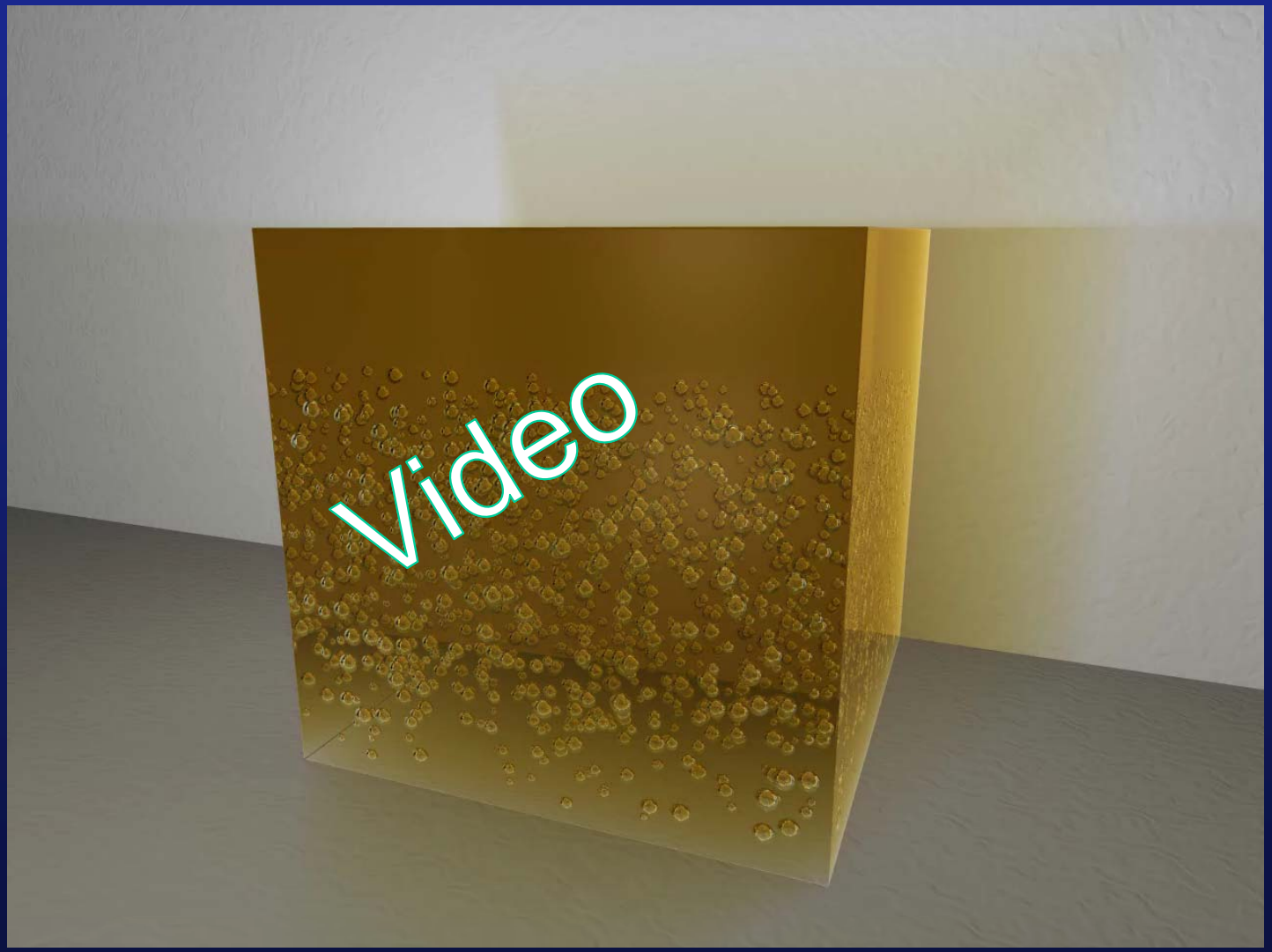
Free-Surface LBM
Bubble Coalescence

- Bubble Coalescence (Bubble Merging)
  - If two bubbles touch each other:
    - Add initial and current volume from bubble with higher index to bubble with lower index

$$V^*_{\min(\mathcal{B})} = \sum_{b \in \mathcal{B}} V^*_b$$
$$V_{\min(\mathcal{B})}(t) = \sum_{b \in \mathcal{B}} V_b(t)$$

    - Delete bubble with higher index
    - Connect all cells belonging to old bubble to new bubble
  - If target bubble merges with other bubble, do process iteratively

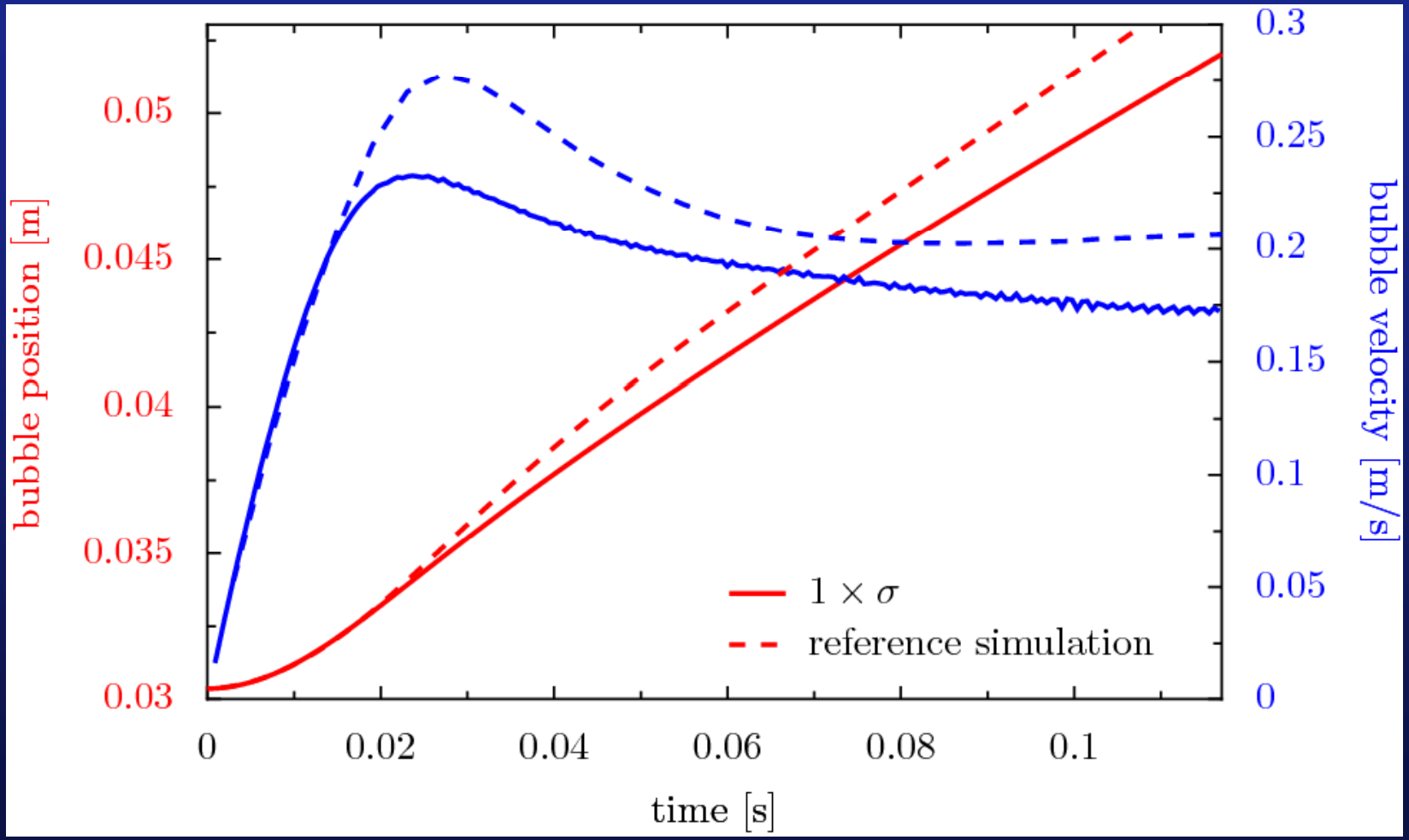
Large-Scale Simulation: 1000 Bubbles



Simulation
- 1000 Bubbles
- 510x510x530 = $1.4 \cdot 10^8$ lattice cells
- 70,000 time steps
- 77 GB
- 64 processes
- 72 hours
- 4,608 core hours

Visualization
- 360 images
- 8 processes for 4 hours per image
- 11,520 core hours

Numerical Experiment: Single Rising Bubble in Oil

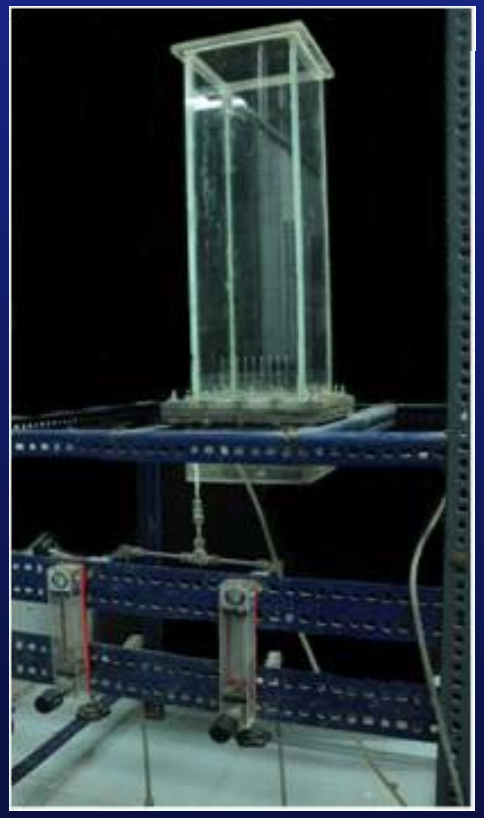


Possible Parameter Range in Free Surface Lattice Boltzmann Method

	Air-Water			Air-Model fluid II			Air-Model fluid III			Air-Model fluid IV		
μ_L	1 x10^{-3} kg/m.s (μ^*_{ref})			μ^*_{ref}			**1 / 50 μ^*_{ref}**			μ^*_{ref}		
ρ_L	1000 kg/m^3(ρ^*_{ref})			ρ^*_{ref}			ρ^*_{ref}			**0.5 / 2ρ^*_{ref}**		
σ_{GL}	0.072 N/m (σ^*_{ref})			**0.5 / 2.0 σ^*_{ref}**			σ^*_{ref}			σ^*_{ref}		
$(dx)_{max}$	6.56x10^{-5} m (=0.065 mm)			1.31x10^{-4} m /3.28x10^{-5} m			6.37x10^{-5} m /0.16 m			3.28x10^{-5} m / 1.31x10^{-4} m		
$(dt)_{max}$	1.47x10^{-5} s			5.89x10^{-5} s / 3.68x10^{-6} s			1.47x10^{-5} s / 1.84 s			3.68x10^{-6} s / 5.89x10^{-6} s		
d_B	1 mm	10 mm	20 mm	1 mm	10 mm	20 mm	1 mm	10 mm	20 mm	1 mm	10 mm	20 mm
Reynolds number $\left(Re = \rho_L \lvert V_R \rvert d_B / \mu_L\right)$	200	2000	4000	200	2000	4000	4 - 200	40-2000	80-4000	100 - 400	1000 - 4000	2000 - 8000
Eotvos number $\left(Eo = g\Delta\rho {d_B}^2 / \sigma\right)$	0.13625	13.625	54.5	0.27 - 0.068	27.25-6.8125	109-27.25	0.136	13.625	54.5	0.068 - 0.2725	6.81 - 27.25	27.25 - 109
Morton or Bond no. $\left(Mo = g\Delta\rho {\mu_L}^4 / {\rho_L}^2\sigma^3\right)$	2.63E-11	2.62E-11	2.62E-11	2.10E-10-3.28E-12	2.10E-10-3.28E-12	2.10E-10-3.28E-12	1.6E-4 - 2.62E-11	1.6E-4 - 2.62E-11	1.6E-4 - 2.62E-11	3.29E-12 2.10E-10	3.29E-12 2.10E-10	3.29E-12 2.10E-10
Lattice cells per diameter	15.22	152.23	304	7.69/30.45	76.99/ 304.45	152.23/ 608.90	Not limited by the lattice surface tension (sufficient cells for accurate curvature calculation!)					
Grid requirement for single bubble simulation (domain $5d_B$ x $5d_B$ x 17.5 d_B)	77* 77* 267 =1.58 x10^6	762* 762* 2664 =1.55 x10^9	1523* 1523* 5328 =1.24 x10^{10}	39*39* 134 / 153*153* 533	381*381* 1332 / 1523* 1523* 5328	762*762* 2664 / 3045* 3045* 10656	Note: Maximum lattice surface tension=0.055x10^{-2} ω=1.9599 Maximum workable memory considered in June 2009.					
Memory requirement	0.81 GB	792 GB	6330 GB	0.1 GB /6.39 GB	9 GB / 6.3 TB	792 GB/ 50.6 TB	**Range of parameter that can be considered in the proposed project:** **μ_L= 1-50μ^*_{ref}, ρ_L= 0.5-2ρ^*_{ref}, σ_L= 0.5-2σ^*_{ref}, d_B=1-20 mm** **Re=100 - 8000** **Eo=0.068 - 109** **Mo=1.31E-11 - 1.6E-4** **log Mo=-10.88 to -3.79**					
Approximate no. of bubbles that could be simulated using ~40 TB of memory* (domain for each bubble is $2d_B$*$2d_B$*$2d_B$)	2.63 x10^6 138^3	2744 14^3	343 7^3	19.4 x10^6 269^3 / 343000 70^3	21952 28^3 / 343 7^3	2744 14^3 / 27 3^3						

Experimental Verification

- Experiments with Rising Bubbles in Liquid Column performed by IIT Delhi (Prof. Vivek Buwa)



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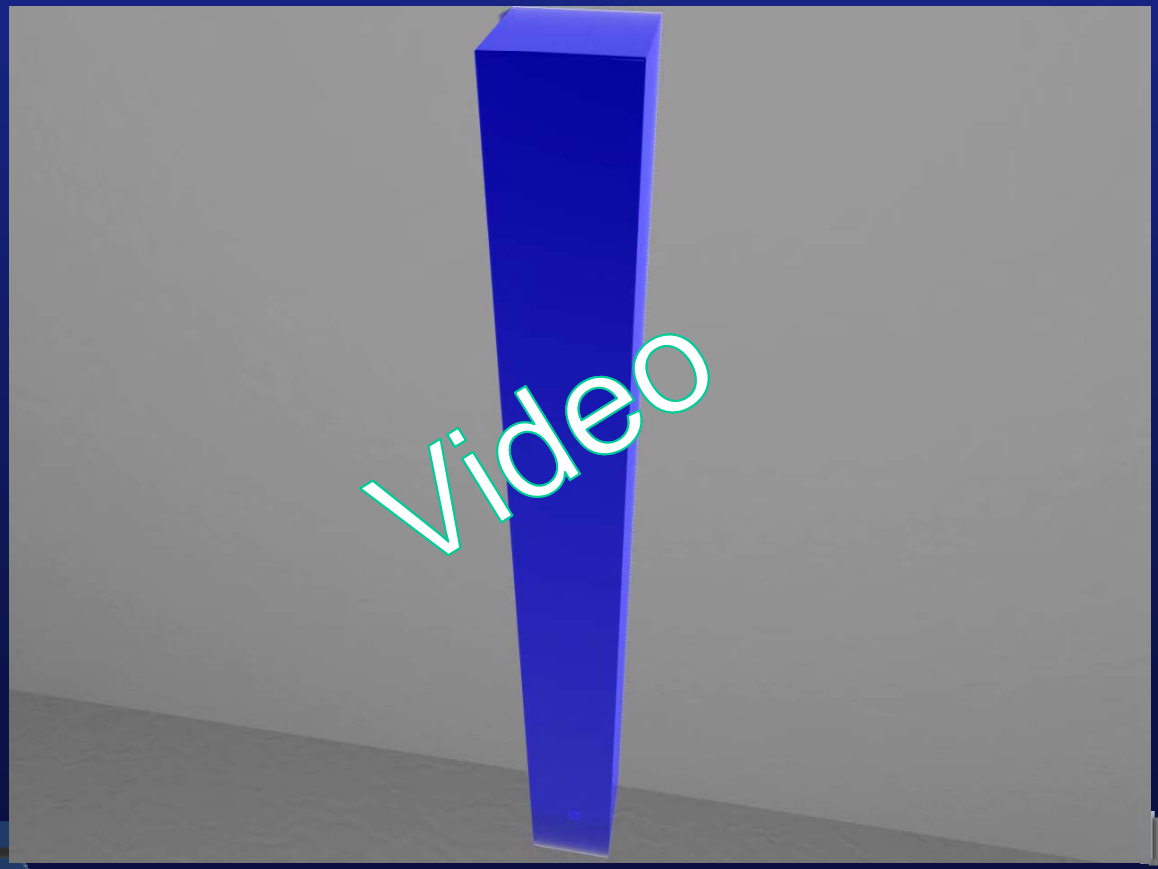
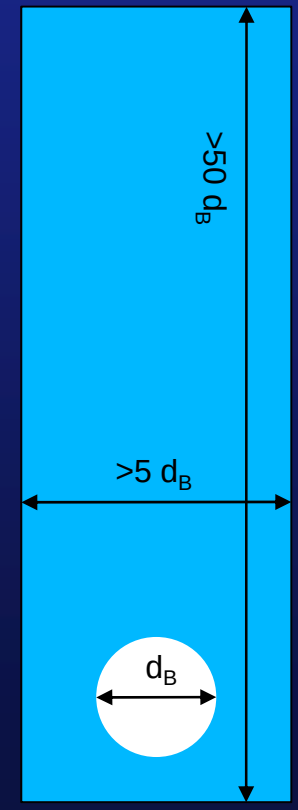
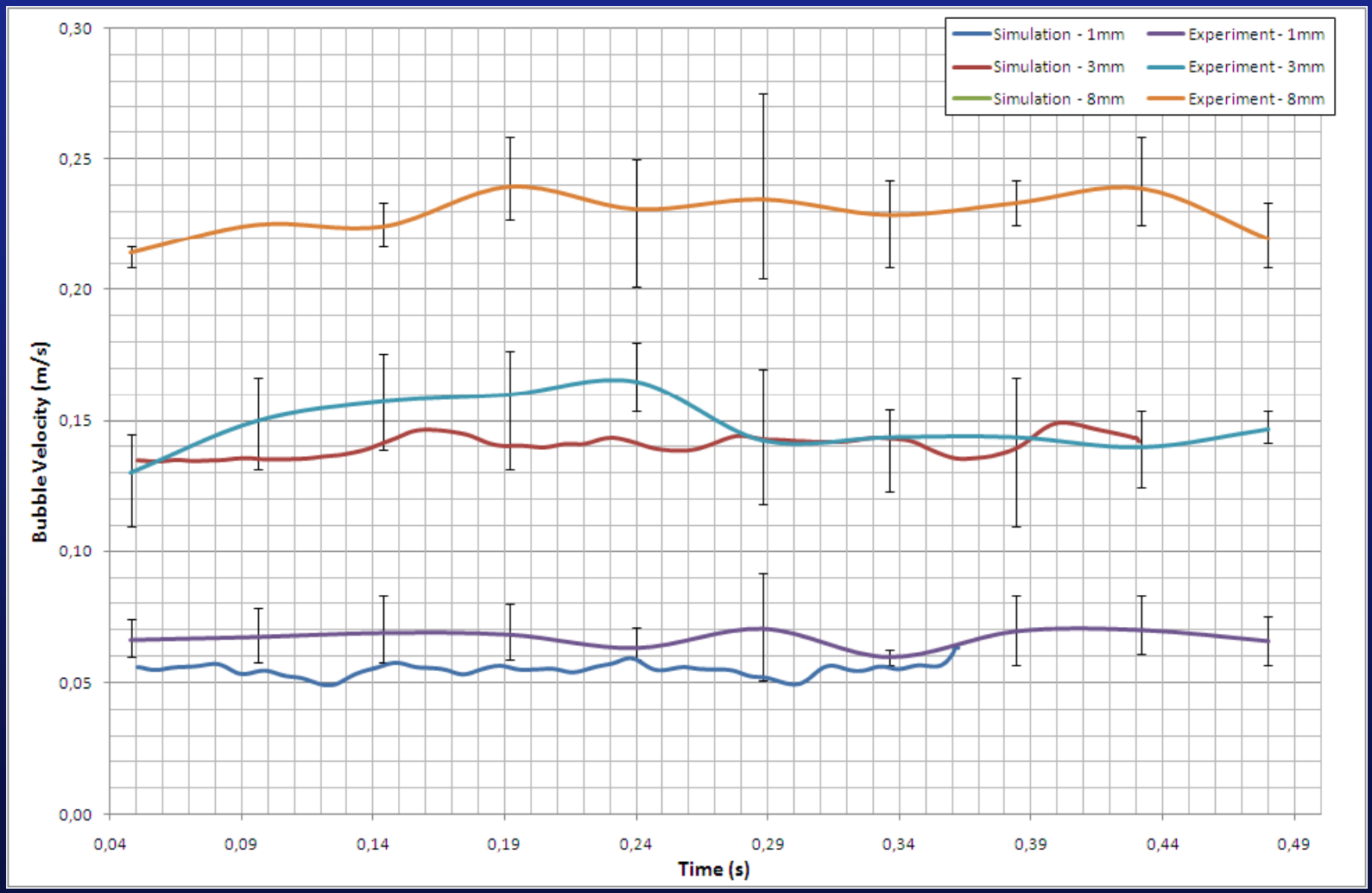




Experimental Verification: Current Results



Conclusion

- Simulation Results Agree Well With Experiments
  - Model is valid and simplifications are justified
  - Surface tension computation is accurate enough
- Efficient Massive-Parallel Two Phase Code Capable of Simulating Real-World Scenarios Correctly
- Outlook: Validation of Multi-Bubble Scenarios

Acknowledgements

- IIT-Delhi for Assessment of Experimental Data
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- Funded by
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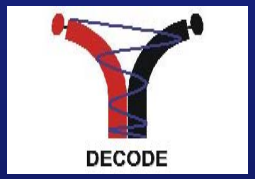
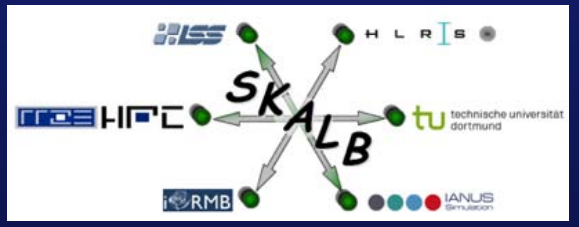
  - KONWIHR, Bavarian project





The End

Thank you for your attention!