# FUNDAMENTAL PRINCIPLES OF THE DISCONTINUOUS GALERKIN METHOD…



TECHNISCHE UNIVERSITÄT DARMSTADT

Dr. Florian Kummer
29th of April, 2021

**Advanced Modeling & Simulation Seminar Series**
**NASA AMES Research Center**

# … AND EXTENSION TO MULTIPHASE FLOW PROBLEMS

MASCHINENBAU
We engineer future FDY

TECHNISCHE UNIVERSITÄT DARMSTADT

# PART 1: FUNDAMENTALS

MASCHINENBAU
We engineer future FDY

# CONTENTS

TECHNISCHE UNIVERSITÄT DARMSTADT


- Introduction
- DG for a scalar conservation law
- Choice of basis
- Tensor basis and fast summation
- Implementation of implicit methods
- Curved/isoparametric elements
- Summary

# BASIC IDEA OF DG

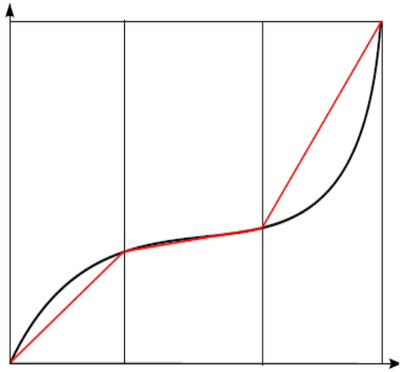
TECHNISCHE UNIVERSITÄT DARMSTADT

- Can be considered a generalization of FVM and FEM
- Higher order, *cell-local* approximation

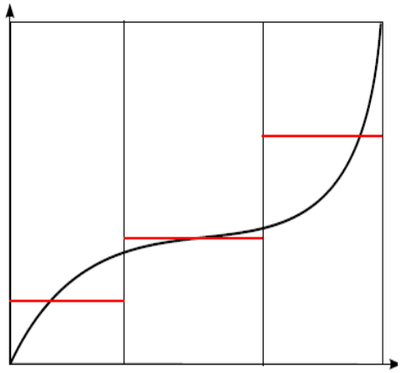
$$u|_K \approx \tilde{u}(x,t) = \sum_{k=1}^{N} \tilde{u}_k(t)\Phi_k(x)$$

Basis polynomials, e.g. $x^2$

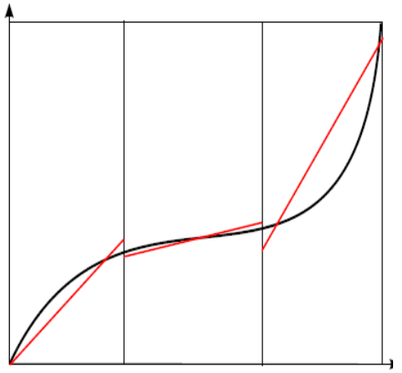
degrees-of-freedom (DG coordinates)



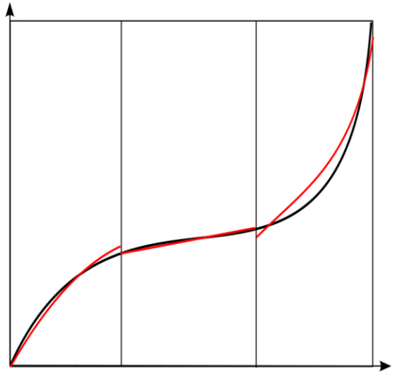
1st order FEM
(continuous)



0th order DG
(= Finite Volume)



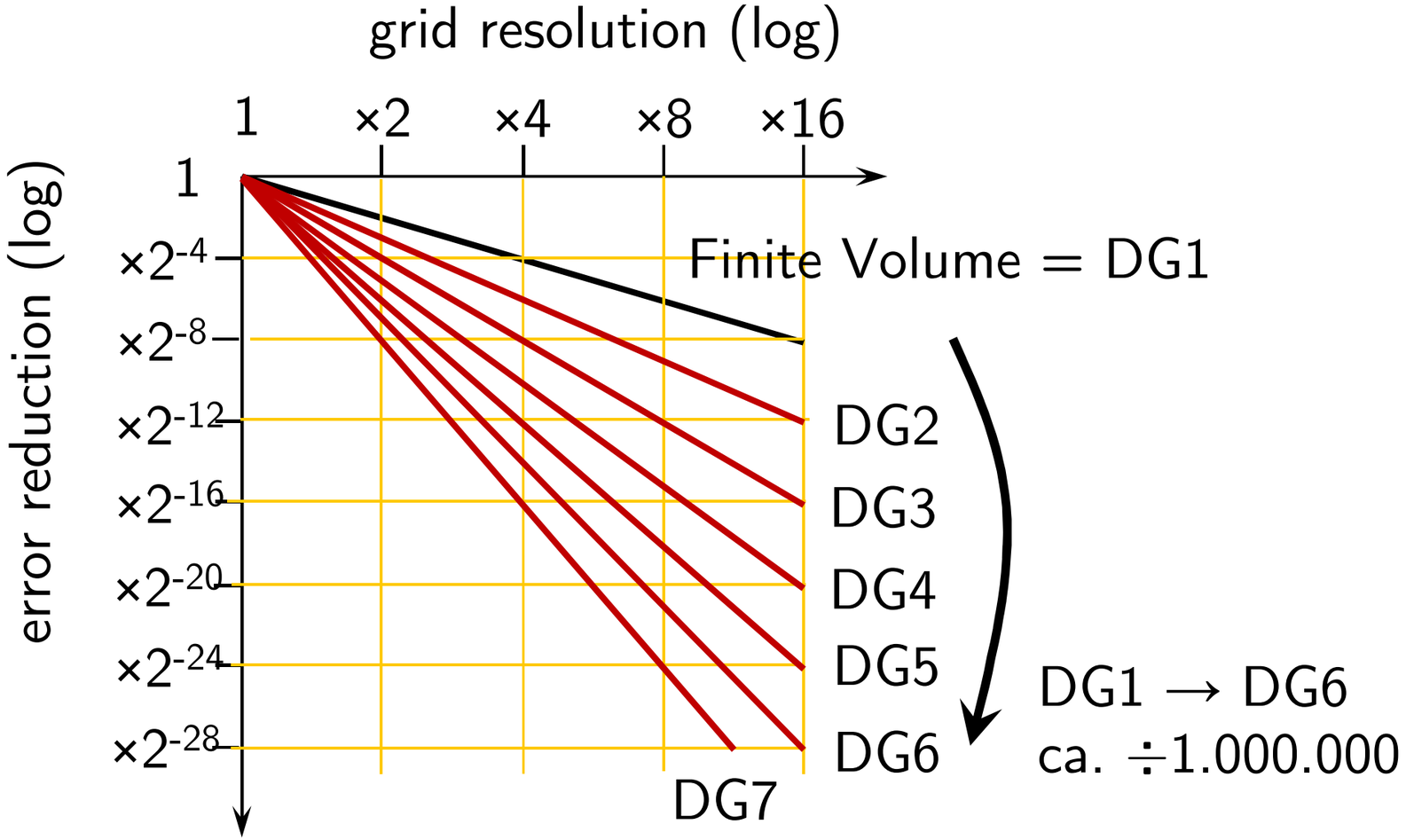
1st order DG
(linear)



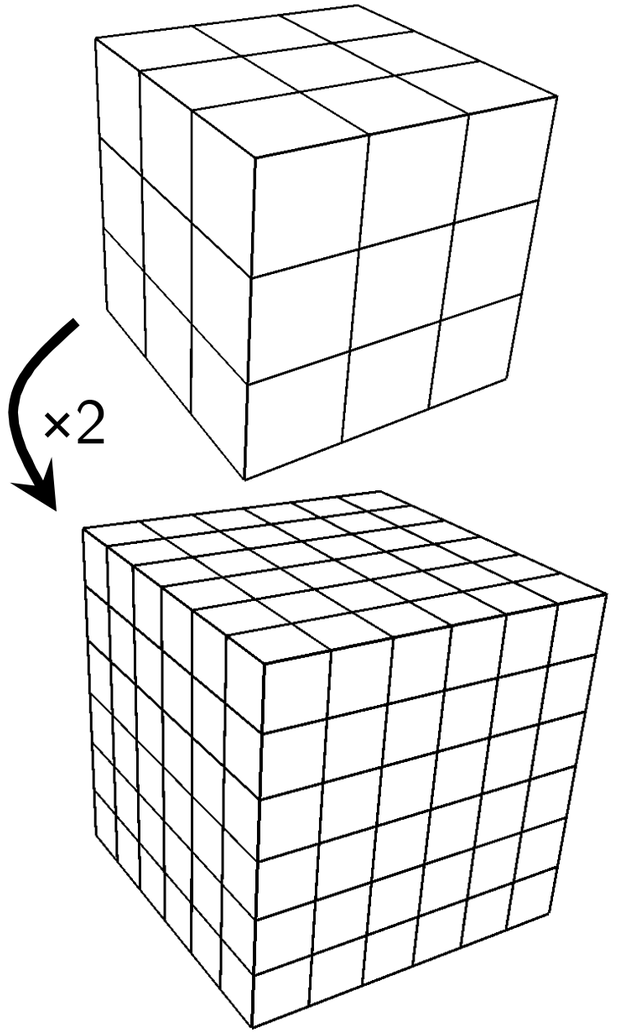
2nd order DG
(quadratic)

# WHY DG? (CONVERGENCE ORDER)

TECHNISCHE UNIVERSITÄT DARMSTADT

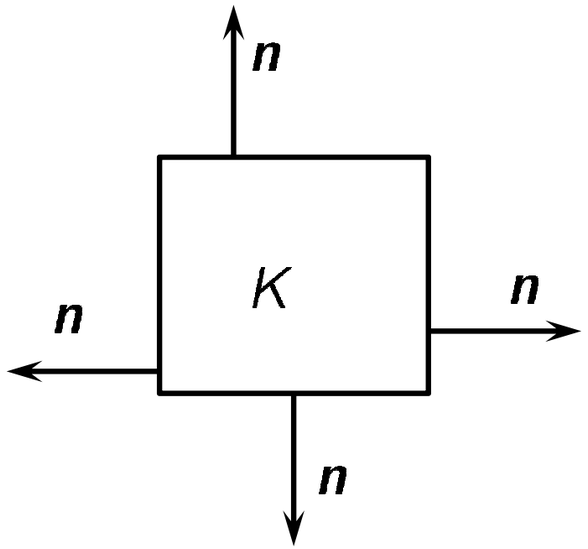



(resolution ×2, 3D → number of cells ×8)



# DG METHOD FOR A SINGLE CELL






$$\partial_t u + \mathrm{div}(\boldsymbol{f}(u)) = 0$$

$$u_h(\boldsymbol{x}, t) = \sum_n \phi_n(\boldsymbol{x})\tilde{u}_n(t)$$

$$\Big| \cdot \phi_m, \quad , \int_K \ldots \mathrm{dV}$$

$$\sum_n \left[ (\partial_t \tilde{u}_n) \int_K \phi_n \phi_m \mathrm{dV} \right] + \int_K \mathrm{div}(\boldsymbol{f}(\sum_n \phi_n \tilde{u}_n))\phi_m \ \mathrm{dV} = 0$$

$$\sum_n [\partial_t \tilde{u}_n \ M_{mn}] + \oint_{\partial K} \underbrace{\boldsymbol{f}(u_h) \cdot \boldsymbol{n}}_{=\hat{f} \text{ (num. flux)}} \ \phi_m \ \mathrm{dS} - \int_K \boldsymbol{f}(u_h) \cdot \nabla \phi_m \ \mathrm{dV} = 0$$

# IMPLEMENTATION OF THE VOLUME TERM

TECHNISCHE UNIVERSITÄT DARMSTADT

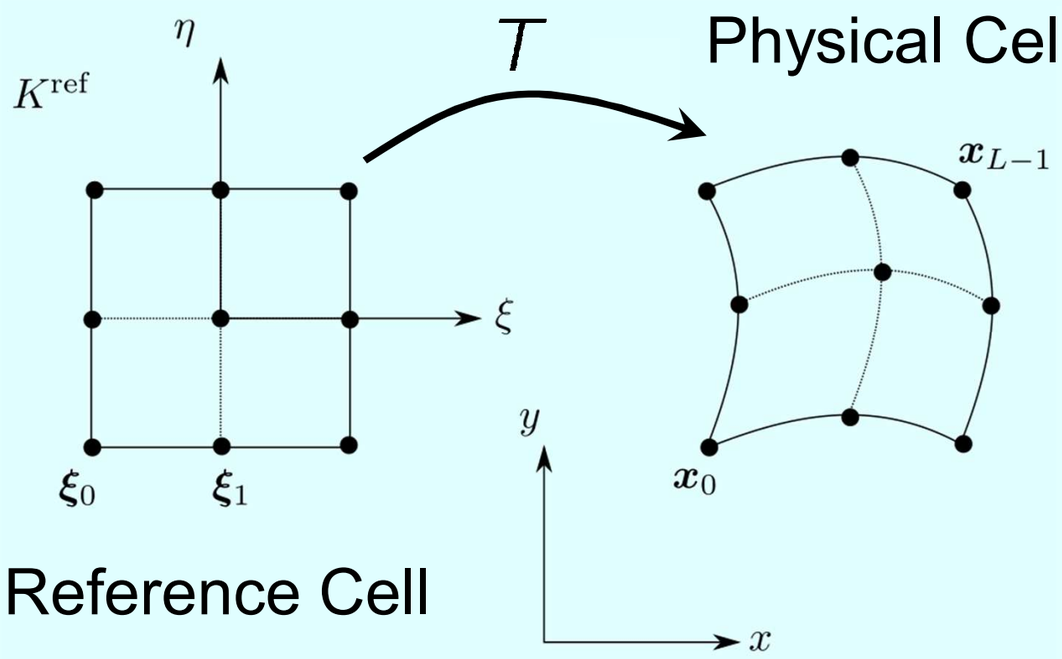
$$\sum_n \left[\partial_t \tilde{u}_n \; M_{mn}\right] + \oint_{\partial K} \underbrace{\boldsymbol{f}(u_h)\cdot\boldsymbol{n}}_{=\hat{f}\ \text{(num. flux)}} \; \phi_m \; \mathrm{dS} - \underbrace{\int_K \boldsymbol{f}(u_h)\cdot\nabla\phi_m \; \mathrm{dV}}_{=F_m^{\mathrm{vol}}} = 0$$

Integral Transformation:

$$\int_K g(\boldsymbol{x}) \; \mathrm{d}\boldsymbol{x} = \int_{K^{\mathrm{ref}}} g(T(\boldsymbol{\xi}))\left|\det(\nabla T(\boldsymbol{\xi}))\right| \; \mathrm{d}\boldsymbol{\xi}$$

Numerical Integration/Quadrature:

$$\int_{K^{\mathrm{ref}}} h(\boldsymbol{\xi}) \; \mathrm{d}\boldsymbol{\xi} \approx \sum_k w_k \, h(\boldsymbol{\xi}_k)$$



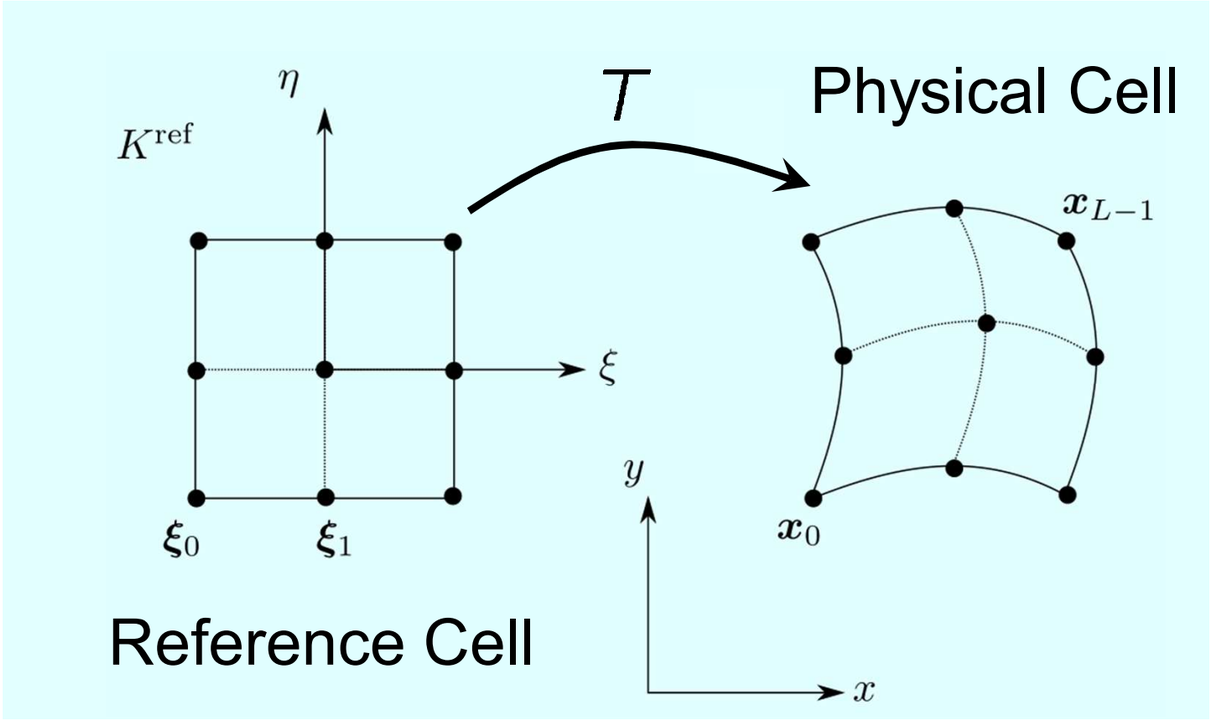
# IMPLEMENTATION OF THE VOLUME TERM

TECHNISCHE UNIVERSITÄT DARMSTADT

$$F_m^{\text{vol}} = \int_K \boldsymbol{f}(u_h) \cdot \nabla \phi_m \, \mathrm{dV}$$

$$= \int_{K^{\text{ref}}} \boldsymbol{f}(u_h) \cdot \nabla \phi_m |\det(\nabla T(\boldsymbol{\xi}))| \, \mathrm{d}\boldsymbol{\xi}$$

$$\approx \sum_{k=1}^{L} w_k \boldsymbol{f}(u_h(\boldsymbol{x}_k)) \cdot \nabla \phi_m(\boldsymbol{x}_k) |\det(\nabla T(\boldsymbol{\xi}_k))|$$



# IMPLEMENTATION OF THE VOLUME TERM

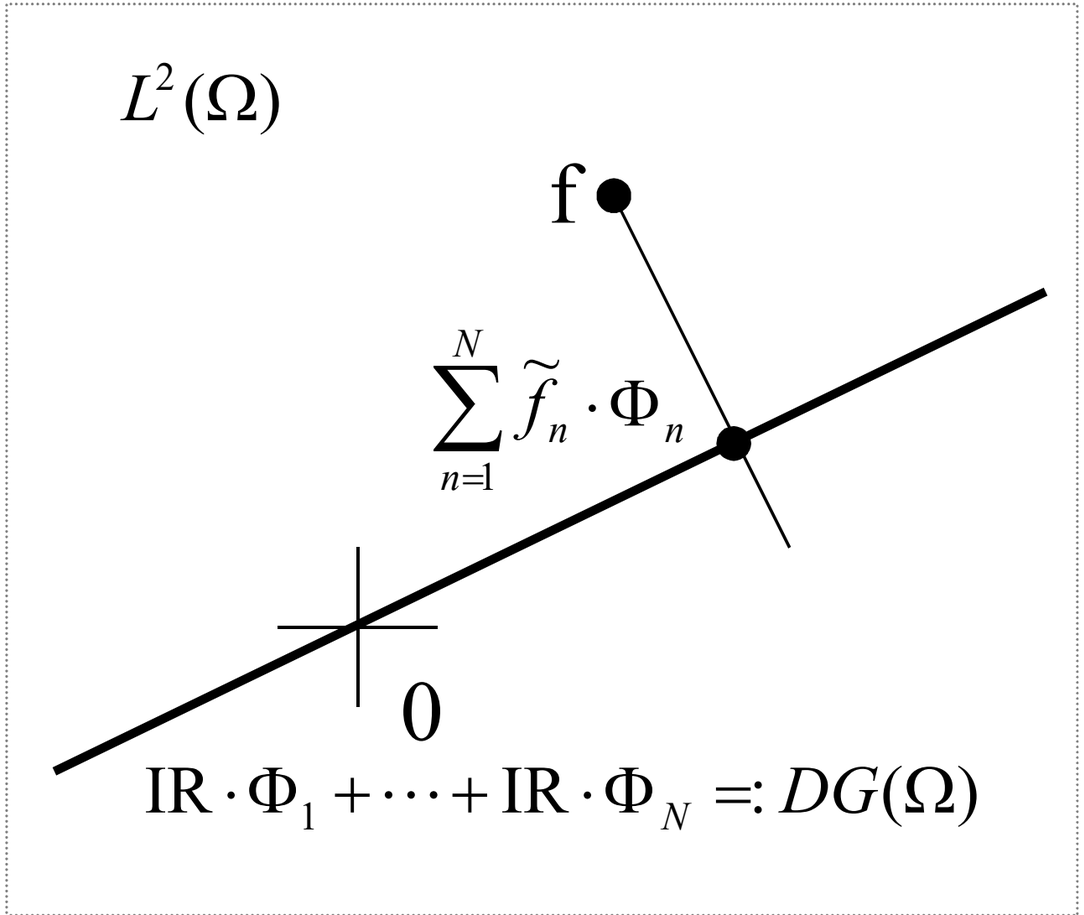
TECHNISCHE UNIVERSITÄT DARMSTADT

1. Evaluate DG at quad. points $\boldsymbol{\xi}_1, \cdots, \boldsymbol{\xi}_L$: $u_h(\boldsymbol{x}_k)$
2. Evaluate fluxes at quad. points: $\boldsymbol{f}(u_h(\boldsymbol{x}_k))$
3. Evaluate integral metrics $|\det(\nabla T(\boldsymbol{\xi}_k))|$
4. Evaluate volume terms $F_1^{\text{vol}}, \ldots, F_M^{\text{vol}}$

$$
\begin{aligned}
F_m^{\text{vol}} &= \int_K \boldsymbol{f}(u_h) \cdot \nabla \phi_m \, \mathrm{dV} \\
&= \int_{K^{\text{ref}}} \boldsymbol{f}(u_h) \cdot \nabla \phi_m |\det(\nabla T(\boldsymbol{\xi}))| \, \mathrm{d}\boldsymbol{\xi} \\
&\approx \sum_{k=1}^{L} w_k \boldsymbol{f}(u_h(\boldsymbol{x}_k)) \cdot \nabla \phi_m(\boldsymbol{x}_k) |\det(\nabla T(\boldsymbol{\xi}_k))|
\end{aligned}
$$

# "GALERKIN ORTHOGONALITY"

$$\int_\Omega f(x)\cdot g(x)dx =: (f,g)$$ is a scalar Product on $L^2(\Omega)$




$$\Phi_1, \cdots, \Phi_N$$

$$DG(\Omega)$$

$$(\Phi_n, \Phi_m) = \delta_{n,m}$$

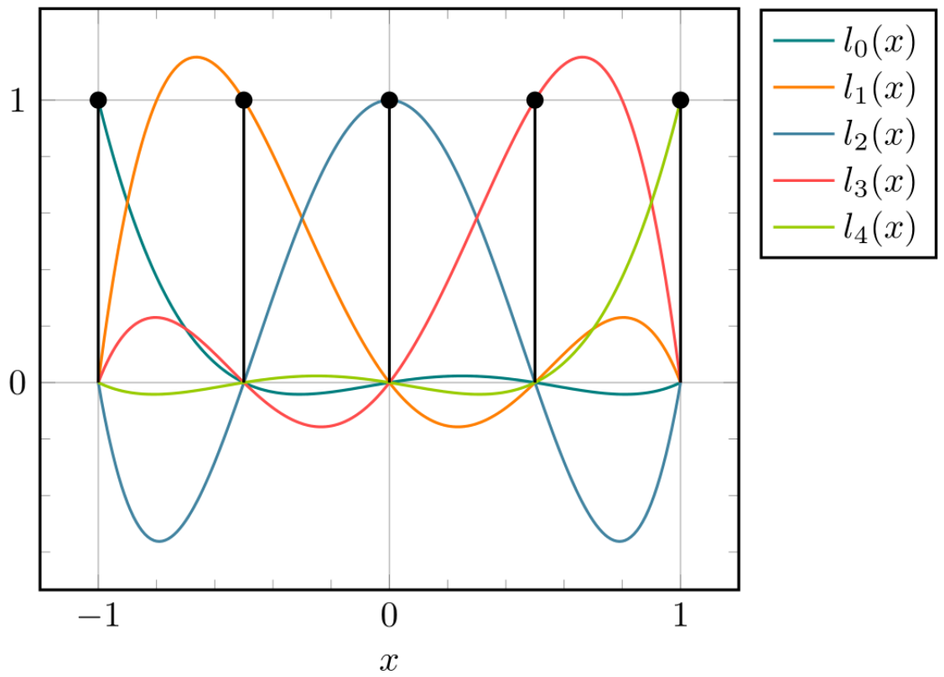
Orthogonal Projection:

$$\tilde{f}_n = (f, \Phi_n)$$

# CHOICE OF BASIS (1D)

TECHNISCHE UNIVERSITÄT DARMSTADT

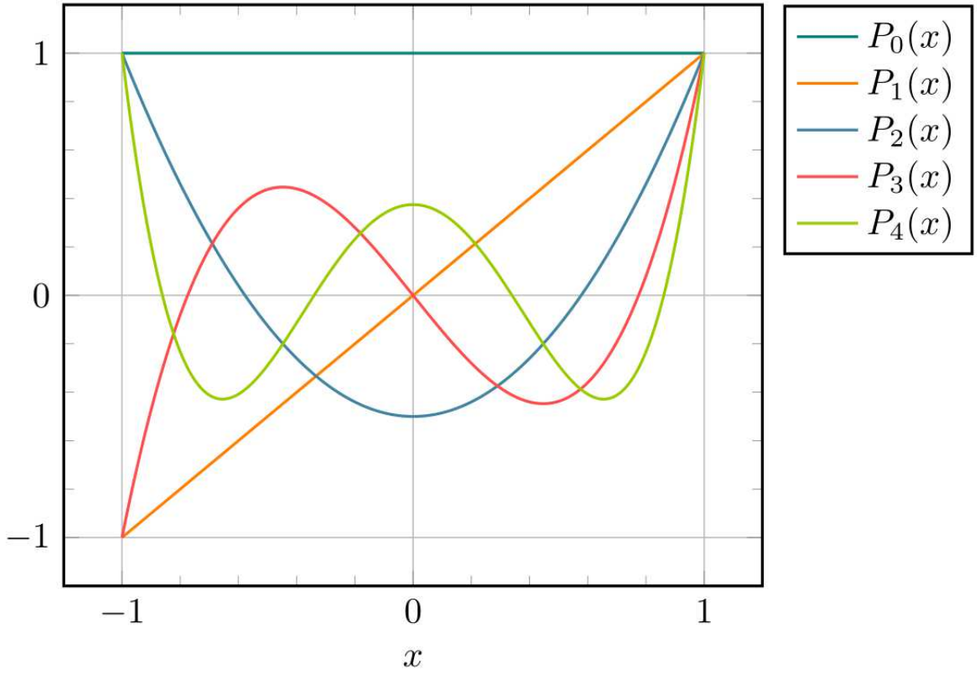
## Nodal Polynomials (Lagrange)




evaluation at nodes is superfast

$$u_h(\boldsymbol{x}_k) = \sum_n \underbrace{\phi_n(\boldsymbol{x}_k)}_{=\delta_{nk}} \tilde{u}_n = \tilde{u}_k$$

## Modal Polynomials (Legendre)




usually orthogonal/orthonormal

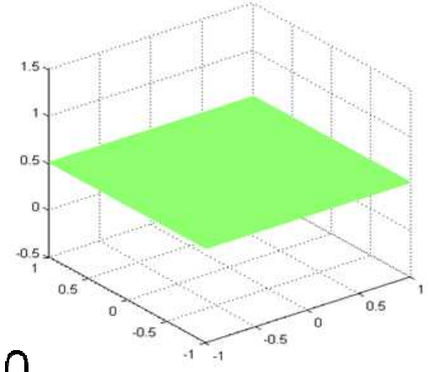
$$M_{mn} = \int_K \phi_n \phi_m \, \mathrm{dV} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases} = I$$

# CHOICE OF BASIS (2D)

TECHNISCHE UNIVERSITÄT DARMSTADT

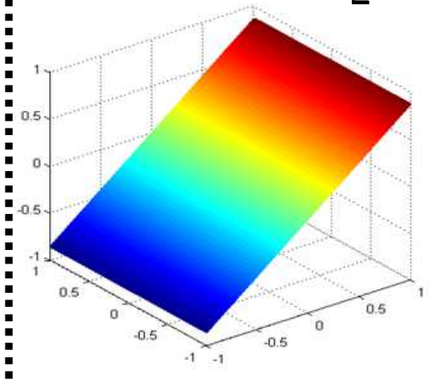
$p = 0$

$\phi_1 = \frac{1}{2}$

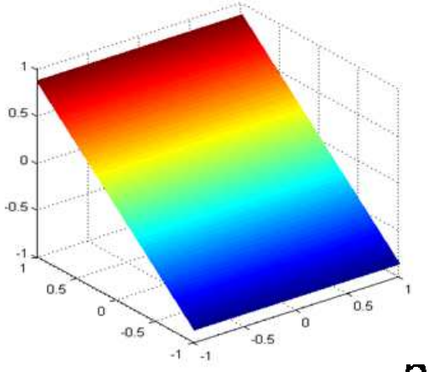


$p = 1$

$\phi_2 = x\frac{\sqrt{3}}{2}$

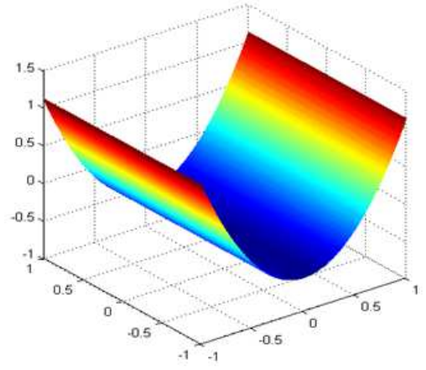


$\phi_3 = y\frac{\sqrt{3}}{2}$

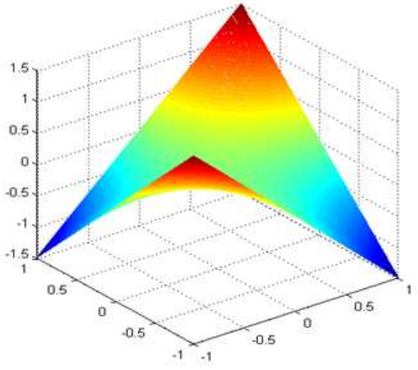


$p = 2$

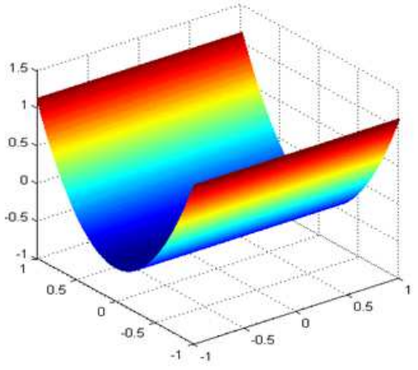
$\phi_4 = \frac{3\cdot\sqrt{5}}{4}x^2 - \frac{\sqrt{5}}{4}$



$\phi_5 = \frac{3}{2}xy$



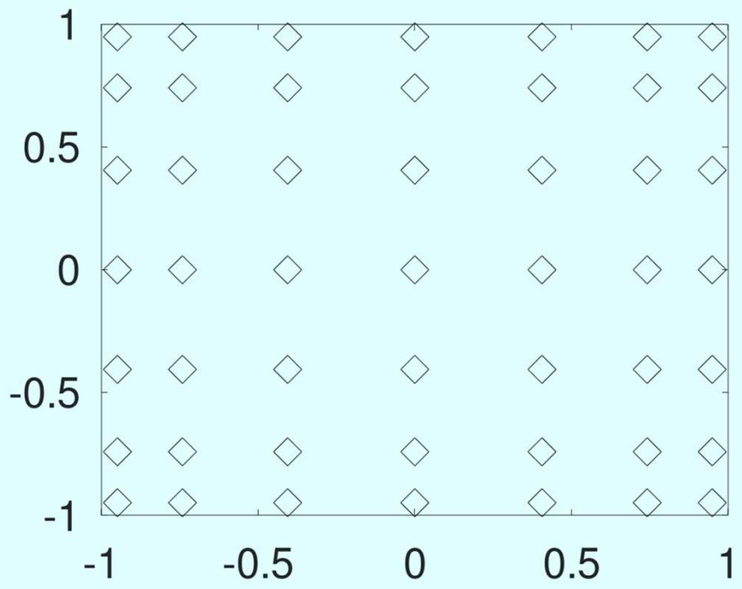
$\phi_6 = \frac{3\cdot\sqrt{5}}{4}y^2 - \frac{\sqrt{5}}{4}$



# NODAL POLYNOMIALS AND QUADRATURE

TECHNISCHE UNIVERSITÄT DARMSTADT

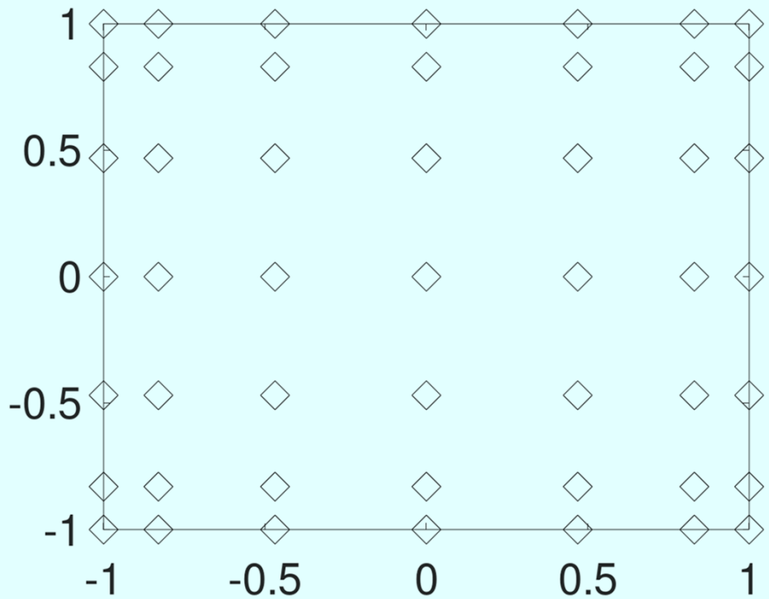
## Gauß-Legendre Quadrature




$N$ nodes $\Rightarrow$ DG polynomial degree $p = N - 1$
quadrature order: $2N - 1 = 2p + 1$

But: requires full evaluation for surface term

## Gauß-Lobatto Quadrature




quadrature order: $2N - 3 = 2p - 1$

already insufficient for linear source terms

# NODAL POLYNOMIALS AND QUADRATURE

TECHNISCHE UNIVERSITÄT DARMSTADT

$$F_m^{\text{vol}} = \int_{K^{\text{ref}}} \underbrace{\underbrace{\underbrace{\boldsymbol{f}(\underbrace{u_h}_{p})}_{\text{e.g. } 2p} \cdot \underbrace{\nabla \phi_m}_{p-1}}_{3p-1} \underbrace{|\det(\nabla T(\boldsymbol{\xi}))|}_{(p-1)D}}_{(3+D)p-2} \, \mathrm{d}\boldsymbol{\xi}$$

Massive under-integration!

$N$ nodes $\Rightarrow$ DG polynomial degree $p = N - 1$
quadrature order: $2N - 1 = 2p + 1$

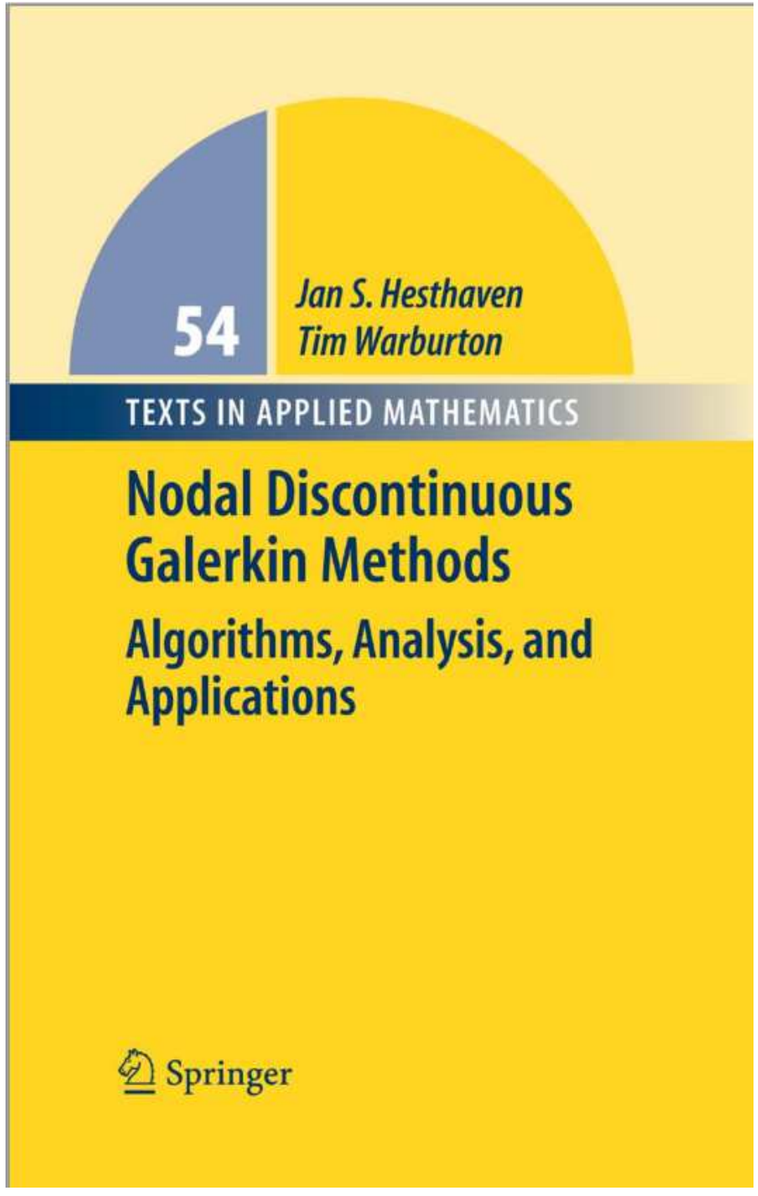
But: requires full evaluation for surface term

quadrature order: $2N - 3 = 2p - 1$

already insufficient for linear source terms

# RECOMMENDATION FOR NODAL IMPLEMENTATION

TECHNISCHE UNIVERSITÄT DARMSTADT




Use the knowledge of experts

# TENSOR BASIS STRUCTURE

TECHNISCHE UNIVERSITÄT DARMSTADT

Assume Structure:

$$\phi_{kl}(\boldsymbol{x}) = \phi_k(x)\phi_n(y)$$

Challenge:

evaluate DG representation on a grid of points $\boldsymbol{x}_{ij} = (x_i, y_j)$

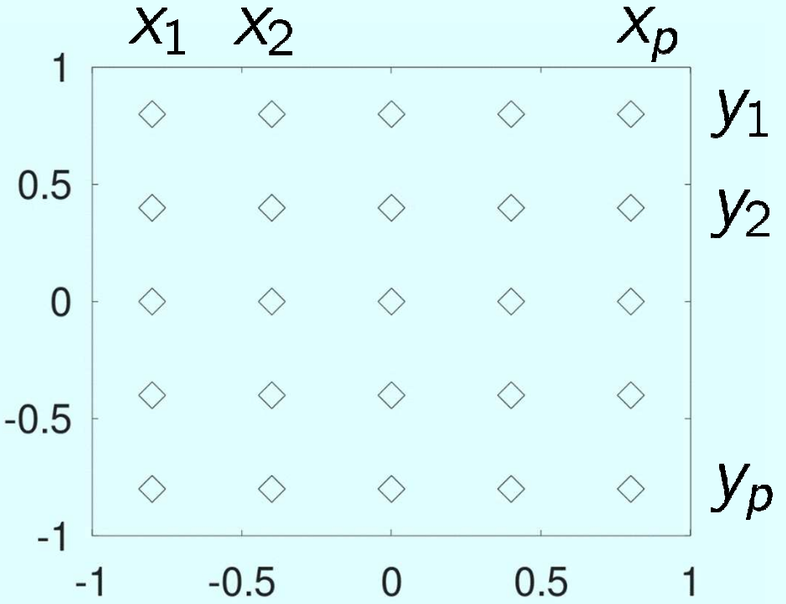
$\mathcal{O}(p)$ For all $i = 1, \ldots, p$:

$\mathcal{O}(p)$ For all $j = 1, \ldots, p$:

$\mathcal{O}(p^2)$

$$u_h(x_i, y_j) = \sum_{k=0}^{p} \sum_{l=0}^{p} \phi_k(x_i)\phi_l(y_j)\tilde{u}_{kl}$$

$\mathcal{O}(p^4)$



# TENSOR BASIS STRUCTURE: FAST SUMMATION

TECHNISCHE UNIVERSITÄT DARMSTADT

$$u_h(x_i, y_j) = \sum_{k=0}^{p} \sum_{l=0}^{p} \phi_k(x_i)\phi_l(y_j)\tilde{u}_{kl}$$

$$= \sum_{k=0}^{p} \phi_k(x_i) \underbrace{\left[ \sum_{l=0}^{p} \phi_l(y_j)\tilde{u}_{kl} \right]}_{=:A_{kj}}$$

2D: $\mathcal{O}(p^4) \rightarrow \mathcal{O}(p^3)$

3D: $\mathcal{O}(p^6) \rightarrow \mathcal{O}(p^4)$

| | |
|---|---|
| $\mathcal{O}(p)$ | For all $k = 1, \ldots, p$: |
| $\mathcal{O}(p)$ | For all $j = 1, \ldots, p$: |
| $\mathcal{O}(p)$ | $A_{kj} = \sum_{l=0}^{p} \phi_l(y_j)\tilde{u}_{kl}$ |
| $\mathcal{O}(p)$ | For all $k = 1, \ldots, p$: |
| $\mathcal{O}(p)$ | For all $j = 1, \ldots, p$: |
| $\mathcal{O}(p)$ | $u_h(x_i, y_j) = \sum_{k=0}^{p} \phi_k(x_i)A_{kj}$ |
| $\mathcal{O}(2p^3)$ | |

# DISCUSSION: TENSOR BASIS & FAST SUMMATION

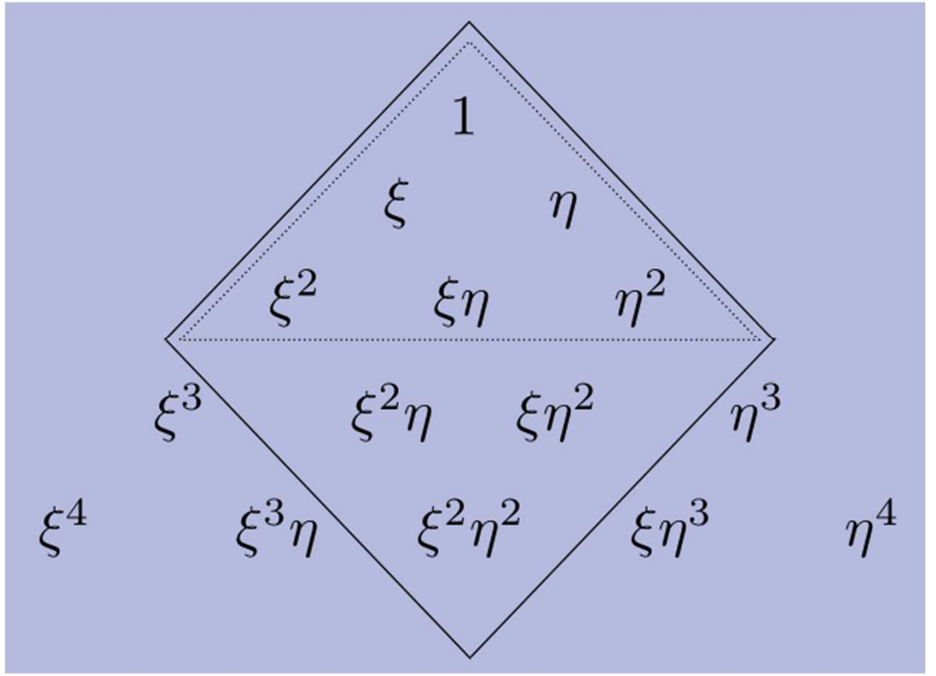
TECHNISCHE UNIVERSITÄT DARMSTADT

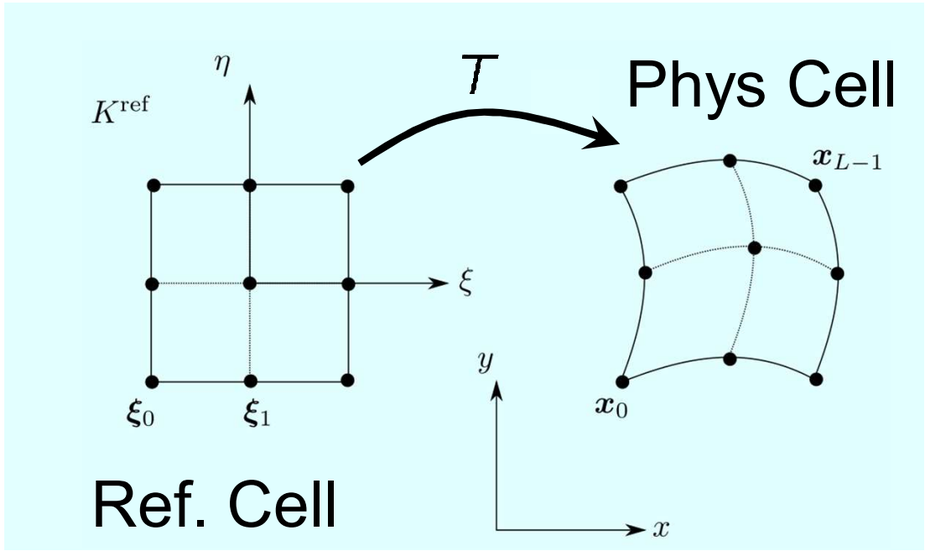
- Applicable for nodal and modal representations
- Essential for performance of **explicit** methods
  - Especially for high polynomial degrees (up to 100)
  - But increases DOF's: not ideal for implicit methods
- Can be applied on all other operations too
  - Volume Terms
  - Surface/Flux Terms
- Difficult for triangles and tetrahedrons

  [Beuchler et.al.: Fast summation techniques for sparse shape functions in tetrahedral hp-FEM, 2013, Lecture Notes in Computational Science and Engineering, Vol 91, Springer, Berlin, Heidelberg.]
  - Works better for quad/hex meshes
- Simplest hardware optimization: BLAS GEMM

# NUMERICAL PROPERTIES OF BASES

- Convergence order does not depend on choice of basis
  - consistency, stability and convergence only depend on monomials covered
  - equivalent basis: equivalent method
- Convergence order can suffer from under-integration
- Exception: tensor bases span a different vector space than modal bases
- Orthonormality of basis breaks under transformation
  - Re-orthonormalize in physical space
  - Work with non-id mass matrix
  - Clever non-linear scaling
  - Ignore through under-integration



# IMPLICIT METHODS (POISSON EQ)

TECHNISCHE UNIVERSITÄT DARMSTADT

E.g. Poisson Equation (strong form):

$$\begin{cases} -\Delta u &= g_\Omega & \text{in } \Omega & \\ u &= g_D & \text{on } \Gamma_D & \text{Dirichlet-boundary} \\ \nabla u \cdot \boldsymbol{n}_{\partial\Omega} &= g_N & \text{on } \Gamma_N & \text{Neumann-boundary} \end{cases}$$

E.g. Poisson Equation (weak form/continuous):

$$\text{Find } u \text{ so that:} \quad a(u,v) = b(v) \quad \text{for all } v$$

$$a(u,v) := \int_\Omega \nabla u \cdot \nabla v \, dV.$$

# IMPLICIT METHODS (POISSON EQ)

TECHNISCHE UNIVERSITÄT DARMSTADT

E.g. Poisson Equation (weak form/continuous):

$$\text{Find DG approx. } u_h \text{ so that: } \quad a_{\text{sip}}(u_h, v_h) = b(v_h) \quad \text{for all } v_h$$

$$a_{\text{sip}}(u,v) = \int_\Omega \underbrace{\nabla u \cdot \nabla v}_{\text{Volume term}} \, dV - \oint_{\Gamma \setminus \Gamma_N} \underbrace{\{\nabla u\} \cdot n_\Gamma \, [\![v]\!]}_{\text{consistency term}} + \underbrace{\{\nabla v\} \cdot \boldsymbol{n}_\Gamma \, [\![u]\!]}_{\text{symmetry term}} \, dA + \oint_{\Gamma \setminus \Gamma_N} \underbrace{\eta \, [\![u]\!] \, [\![v]\!]}_{\text{penalty term}} \, dA$$

$$\underbrace{\begin{bmatrix} a_{\text{sip}}(\Phi_{0,0}, \Phi_{0,0}) & \cdots & a_{\text{sip}}(\Phi_{J-1,N_{P-1}}, \Phi_{0,0}) \\ \vdots & \vdots & \vdots \\ a_{\text{sip}}(\Phi_{0,0}, \Phi_{J-1,N_{P-1}}) & \cdots & a_{\text{sip}}(\Phi_{J-1,N_{P-1}}, \Phi_{J-1,N_{P-1}}) \end{bmatrix}}_{=:\underline{\underline{M}}_{\text{sip}}} \cdot \underbrace{\begin{bmatrix} \tilde{u}_{0,0} \\ \vdots \\ \tilde{u}_{J-1,N_p-1} \end{bmatrix}}_{=:\tilde{u}} = \underbrace{\begin{bmatrix} \int g_\Omega \cdot \Phi_{0,0} \, dV \\ \vdots \\ \int g_\Omega \cdot \Phi_{J-1,N_p-1} \, dV \end{bmatrix}}_{=:\tilde{g}}$$

# IMPLICIT METHODS (POISSON EQ)

TECHNISCHE UNIVERSITÄT DARMSTADT

E.g. Poisson Equation (weak form/continuous):

$$\text{Find DG approx. } u_h \text{ so that:} \quad a_{\text{sip}}(u_h, v_h) = b(v_h) \quad \text{for all } v_h$$

$$a_{\text{sip}}(u,v) = \int_\Omega \underbrace{\nabla u \cdot \nabla v}_{\text{Volume term}} \, dV - \oint_{\Gamma \setminus \Gamma_N} \underbrace{\{\nabla u\} \cdot n_\Gamma \, [\![v]\!]}_{\text{consistency term}} + \underbrace{\{\nabla v\} \cdot \boldsymbol{n}_\Gamma \, [\![u]\!]}_{\text{symmetry term}} \, dA + \oint_{\Gamma \setminus \Gamma_N} \underbrace{\eta \, [\![u]\!] \, [\![v]\!]}_{\text{penalty term}} \, dA$$

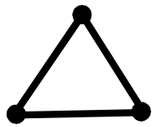
$$\underbrace{\begin{bmatrix} a_{\text{sip}}(\Phi_{0,0}, \Phi_{0,0}) & & \\ \vdots & & \\ \vdots & & \\ a_{\text{sip}}(\Phi_{0,0}, \Phi_{J-1,N_{P-1}}) & \cdots & a_{\text{sip}}(\Phi_{J-1,N_{P-1}}, \Phi_{J-1,N_{P-1}}) \end{bmatrix}}_{=:\underline{\underline{M}}_{\text{sip}}} \underbrace{\begin{bmatrix} \\ \\ \\ u_{J-1,N_p-1} \end{bmatrix}}_{=:\tilde{u}} \underbrace{\begin{bmatrix} \int g_\Omega \cdot \Phi_{0,0} \, dV \\ \vdots \\ \vdots \\ \int g_\Omega \cdot \Phi_{J-1,N_p-1} \, dV \end{bmatrix}}_{=:\tilde{g}}$$

**Programming Challenge:**

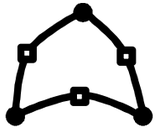
$$a_{\text{sip}}(\Phi_{j,n}, \Phi_{l,m}) = ?$$

# NECESSITY OF ISOPARAMETRIC/CURVED ELEMENTS

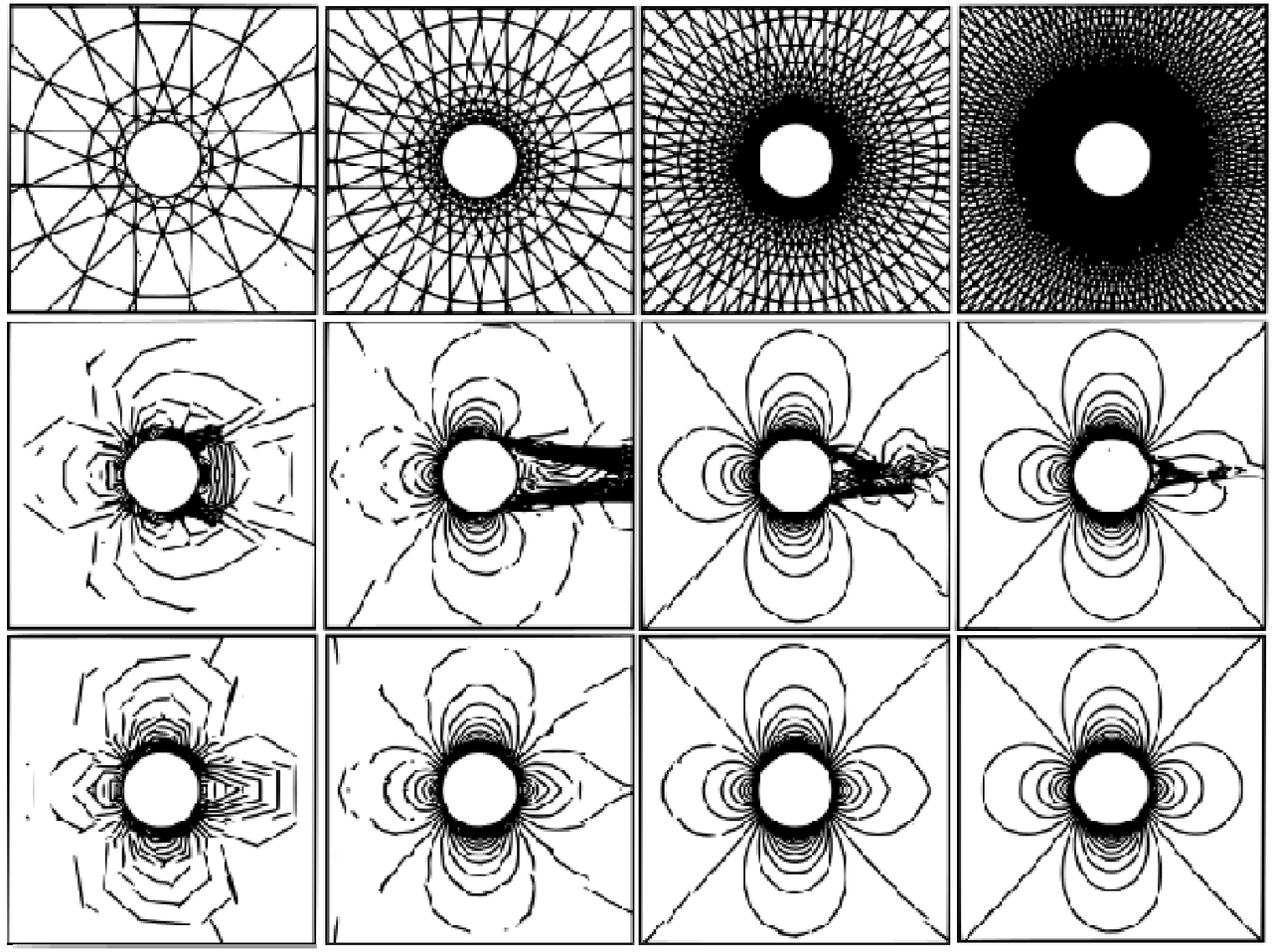
TECHNISCHE UNIVERSITÄT DARMSTADT



Lin. Elm.



Quad. Elm.



$p = 2$ DG simulation,

2D Euler

1st vs. 2nd order elements

[Bassi & Rebay 1997]

Alternative:
IBM/XDG

# CURRENT STATE OF ISOPARAMETRIC ELEMENTS

TECHNISCHE UNIVERSITÄT DARMSTADT

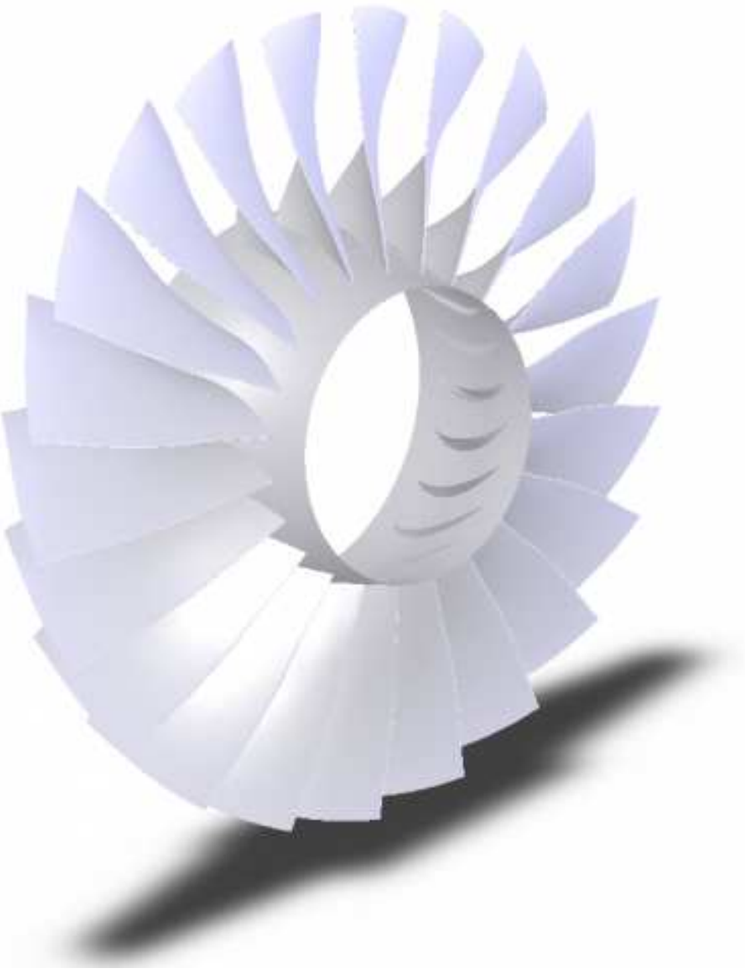
HiOCFD5 | 2018

5th International Workshop on High-Order CFD Methods

**Challenge: NASA Rotor 67**

…**generation of the curved (hybrid) unstructured meshes for a single passage.**

- minimally quadratic interpolation…
- local mesh refinement following size control maps in leakage flow regions;
- curved rotationally periodic boundaries;
- extrusion curved boundary layer meshes…



[https://how5.cenaero.be/content/mc2-nasa-rotor-67]

# SUMMARY OF PART 1

TECHNISCHE UNIVERSITÄT DARMSTADT

- DG methods offer free choice of convergence order
  - Only 1st order fluxes are required
  - E.g. energy-conserving incompressible schemes of arbitrary order
- Choice of basis has an impact on performance, no impact on outcome
- Nodal Implementations
- Acceleration of tensor bases/fast summation
- General idea for implicit methods
- Curved Meshes are absolutly necessary, Tools are still limited

So far, any questions?

TECHNISCHE UNIVERSITÄT DARMSTADT

# *PART 2: MULTIPHASE AND XDG*

# *(THREE PHASE CONTACT LINES)*

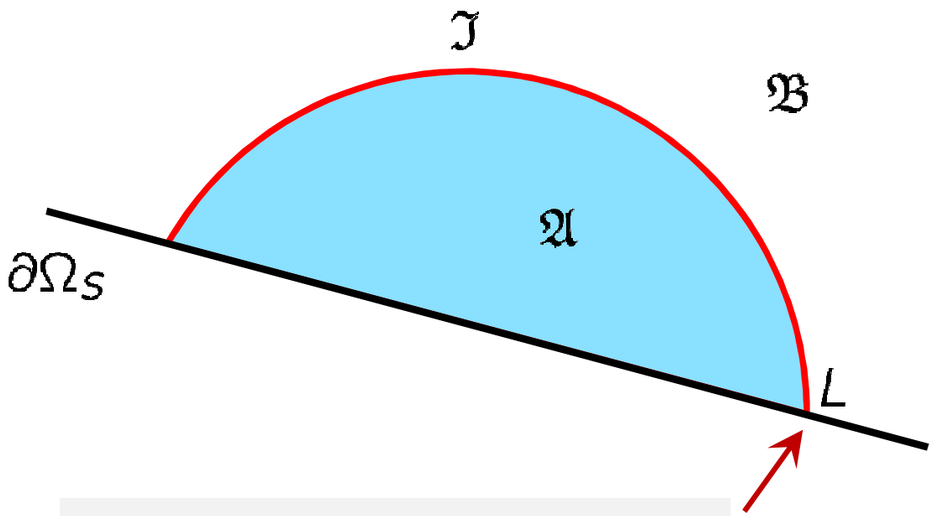
MASCHINENBAU
We engineer future FDY

# CONTENTS

TECHNISCHE UNIVERSITÄT DARMSTADT

- Three-Phase Contact Lines
  - Problem Motivation
  - Mathematical Model
- Extended Discontinuous Galerkin Discretization
- Results

# THREE PHASE CONTACT LINES?




no-slip boundary condition
$\longrightarrow$ no movement
Theoretical analysis by
Huh and Scriven, 1970



www.absfreepic.com

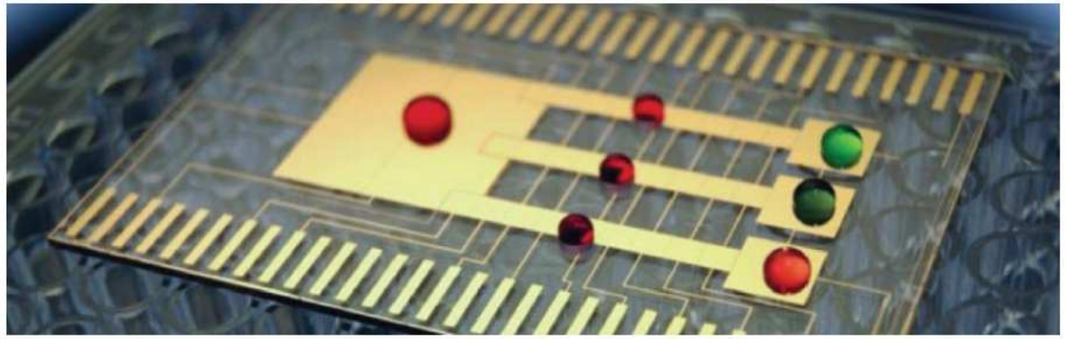
What kind of boundary condition?

Not even Herakles could sink a solid if the physical model [no-slip] were entirely valid !

# TECHNICAL APPLICATIONS

TECHNISCHE UNIVERSITÄT DARMSTADT

- Printing
  (Semiconductor, OLED)
- Coating/painting
  functional Surfaces
- Nano/micro-fluidic devices
  (lab-on-chip)



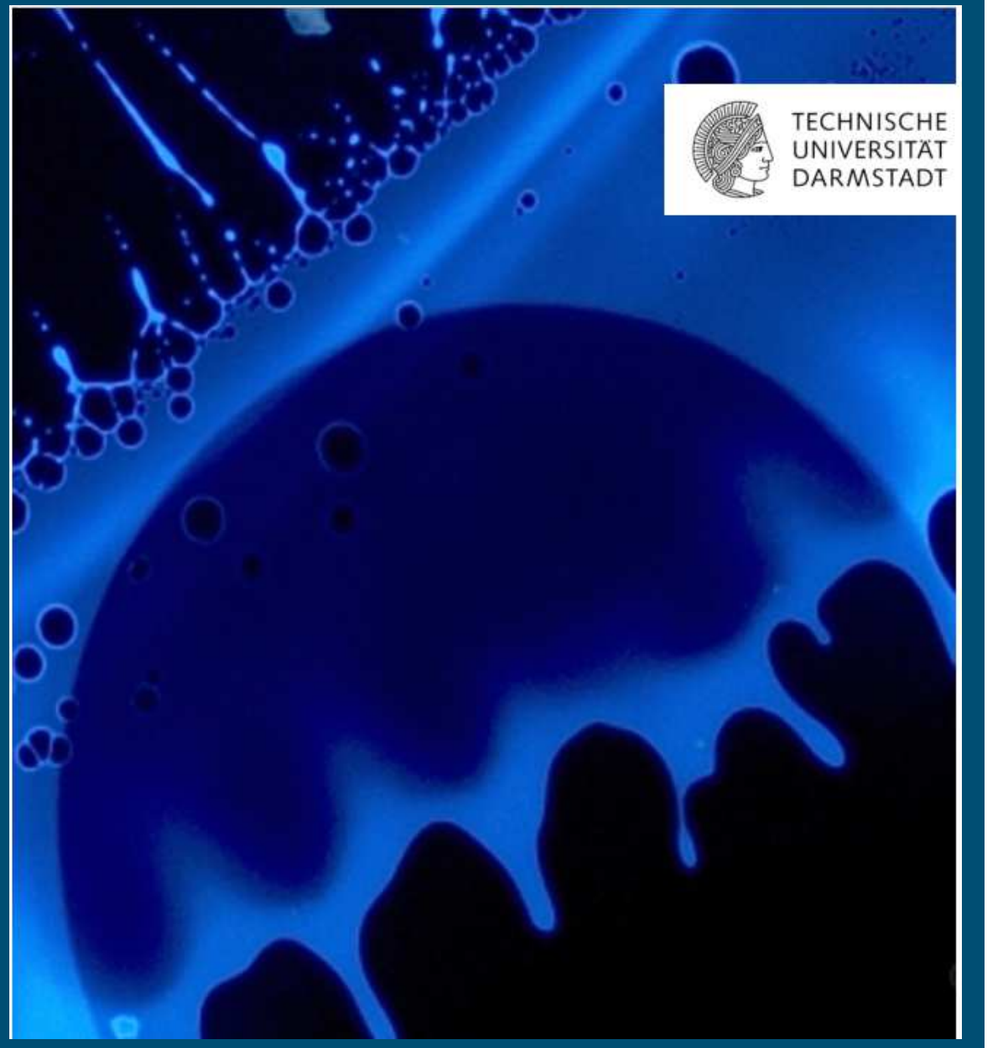




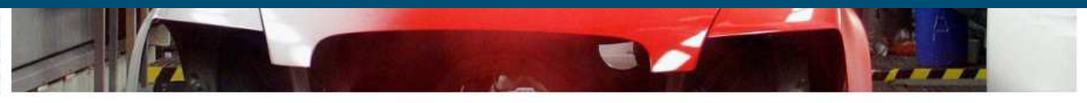
# COLLABORATIVE RESEARCH CENTRE (CRC) 1194

## INTERACTION BETWEEN TRANSPORT AND WETTING PROCESSES

- 20 Projects
- Long-Term Funding: 2016 – 2028
- Go to https://www.sfb1194.tu-darmstadt.de/

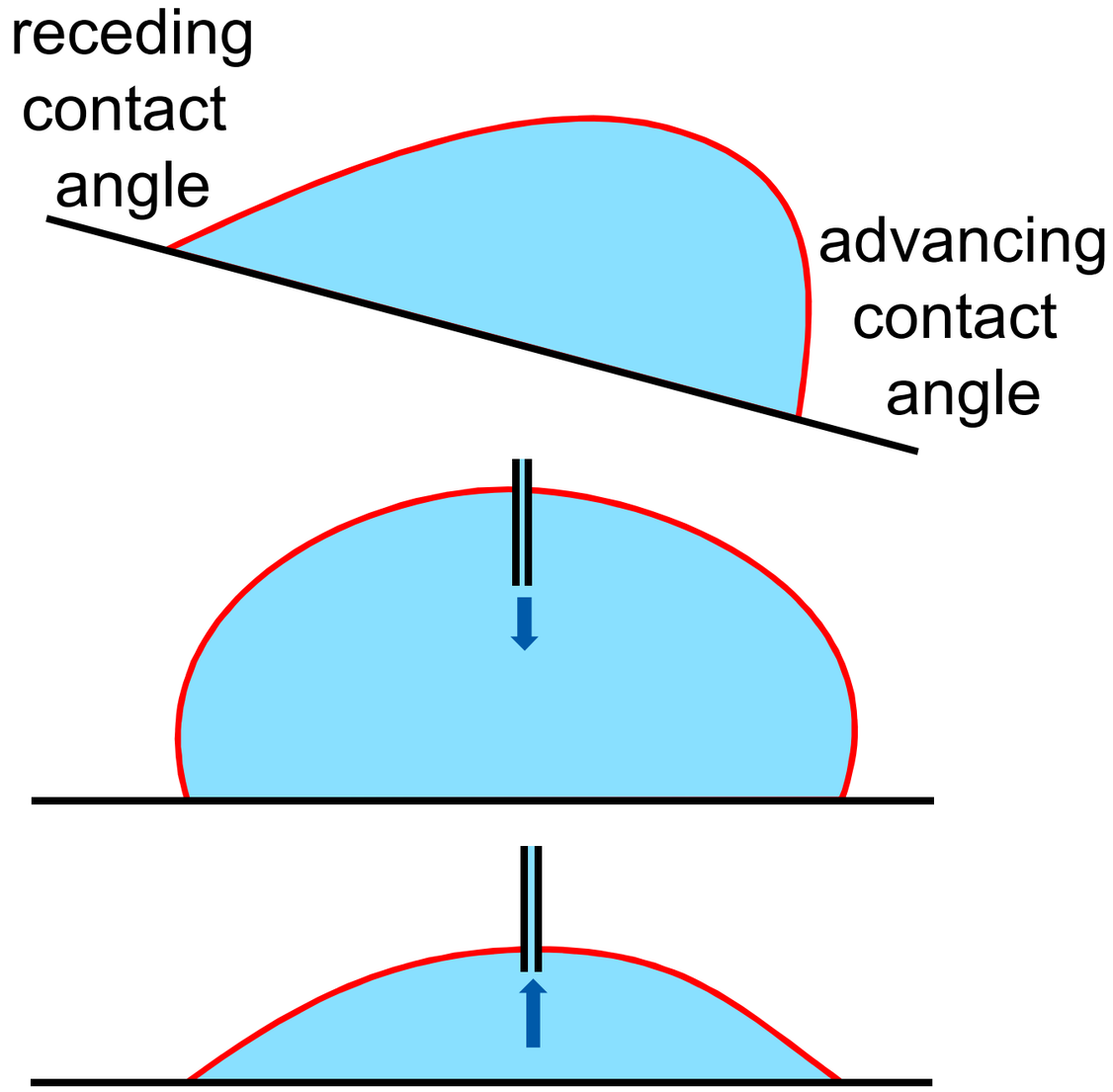




# MATHEMATICAL MODELING

# CONTACT LINE PHENOMENA: ADVANCING & RECEDING ANGLE




- Physical observation
- Hysteresis

  $\Theta_{Rec} \leq \Theta \leq \Theta_{Adv}$

- Creeping & Rolling regime

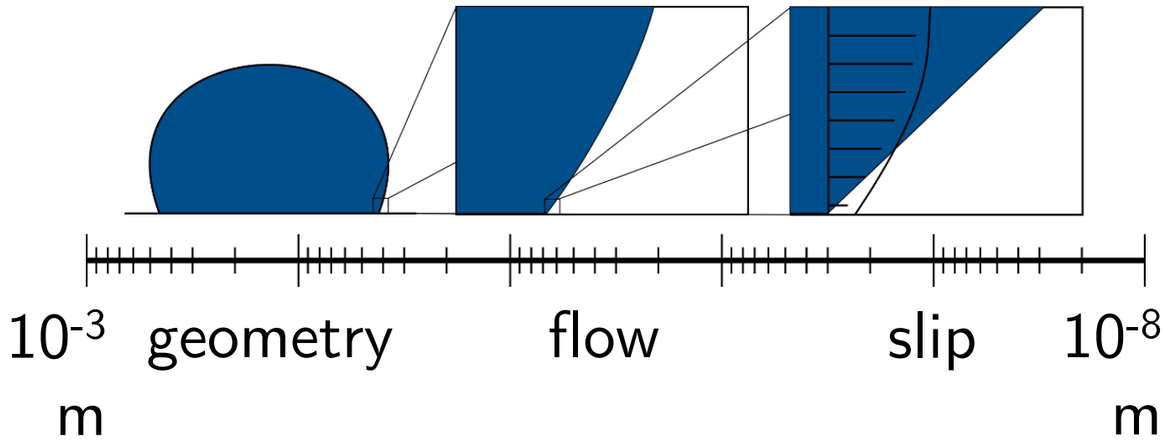
- Still not understood
- molecular dynamics sim. predicts static angle
- beyond continuum physics
- No hysteresis on very clean surfaces
- micro-capillarity?

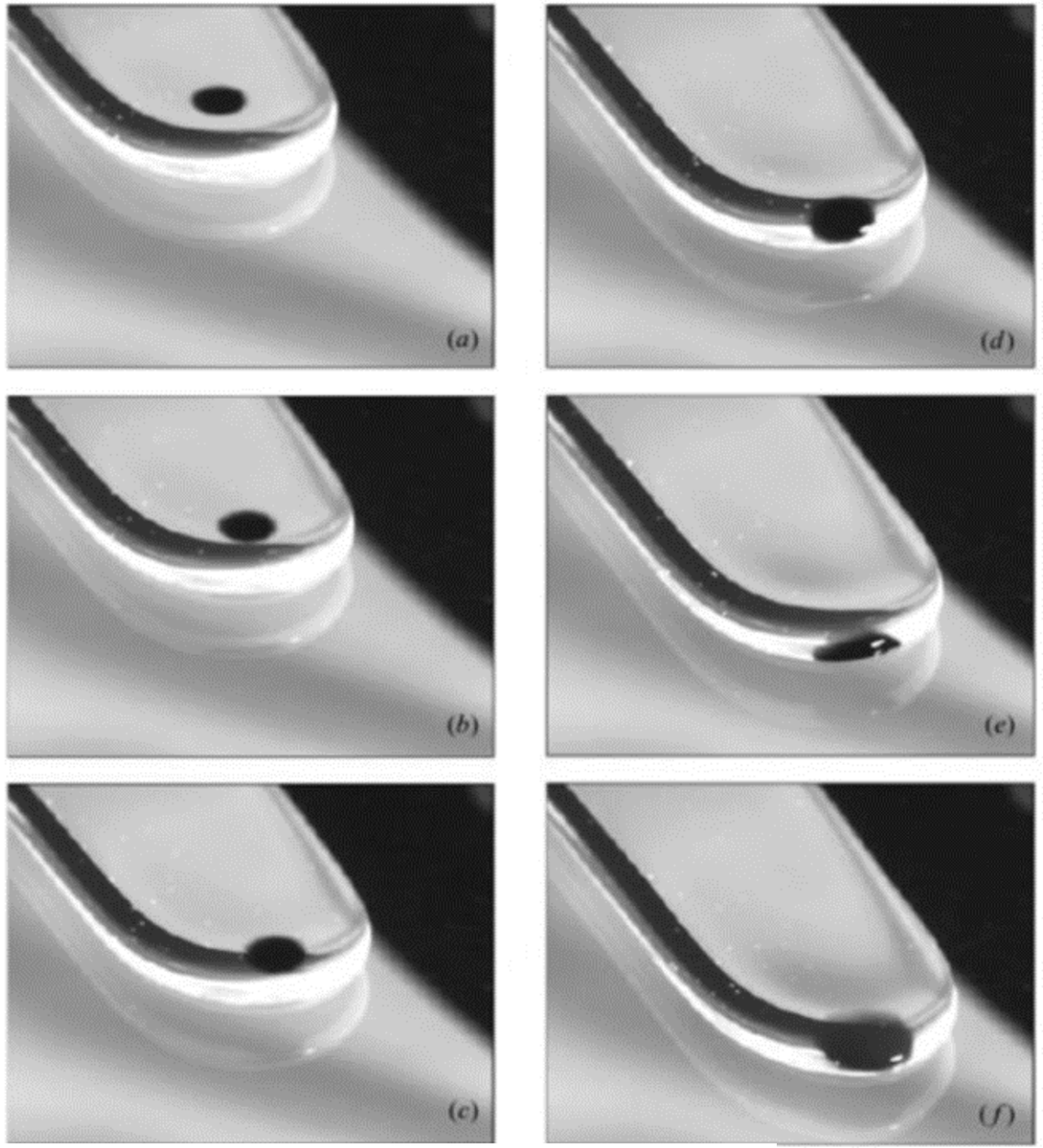
# CONTACT LINE PHENOMENA

- Rolling motion observed in experiments

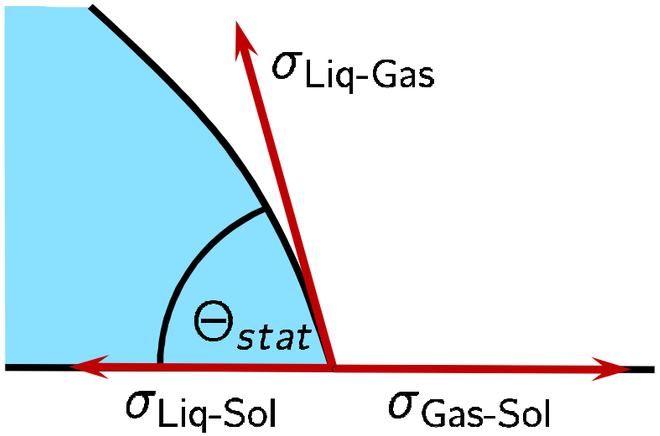
[I. Veretennikov, A. Indeikina, and H.Chang. Front dynamics and fingering of a driven contact line, JFM 373:81-110, 1998]

- Contact line problems involve several magnitudes of length scales



# STATIC CONTACT ANGLE



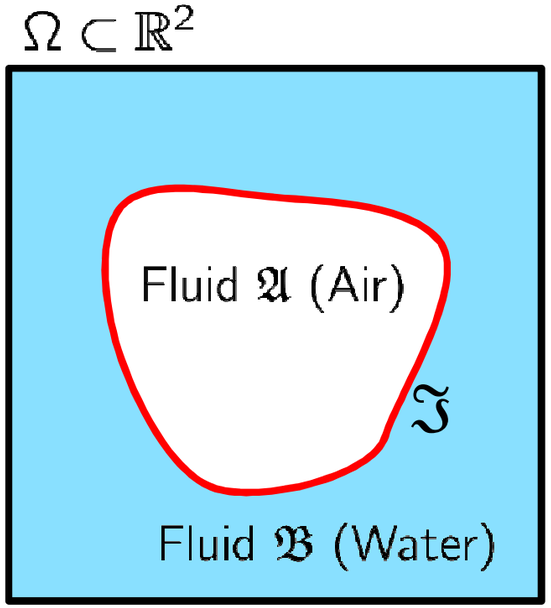

Young's equation:

$$\cos(\Theta_{\text{stat}})\sigma_{\text{Liq-Gas}} + \sigma_{\text{Liq-Sol}} = \sigma_{\text{Gas-Sol}}$$

Static droplet, "sitting" on the surface:

- Balance of forces/tensions in wall-tangential direction

# MATHEMATICAL MODEL FOR TWO PHASES




$\rho$ and $\mu$ are piece-wise constant in $\mathfrak{A}$ and $\mathfrak{B}$

Incompressible Navier-Stokes equations:

$$\frac{\partial}{\partial t}(\rho\vec{u}) + \mathrm{div}(\rho\vec{u}\otimes\vec{u}) + \nabla p = \mu\Delta\vec{u}$$

$$\mathrm{div}(\vec{u}) = 0$$

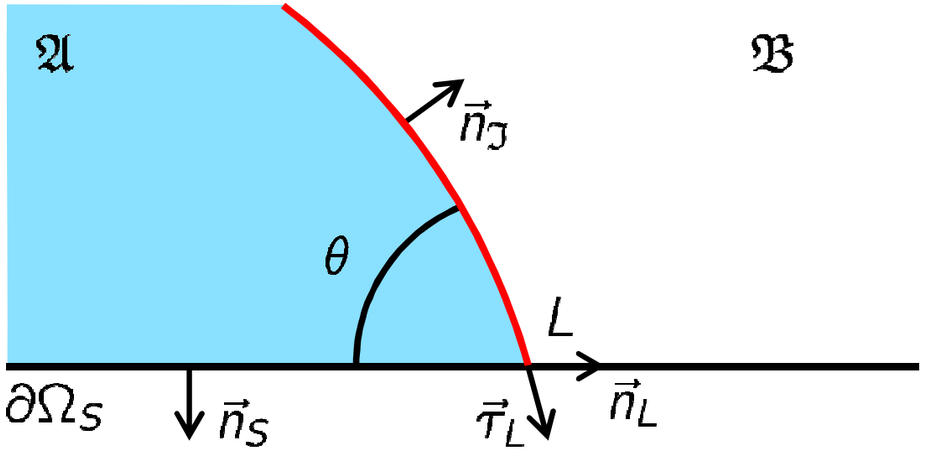
Jump conditions at interface $\mathfrak{I}$:

$$[\![\vec{u}]\!] = 0$$

$$[\![p\vec{n} - \mu(\nabla\vec{u} + \nabla\vec{u}^T)\vec{n}]\!] = \sigma\kappa\vec{n}$$

surface tension
local curvature
interface normal

# MATHEMATICAL MODEL FOR CONTACT LINE: GENERALIZED NAVIER BOUNDARY CONDITION




Wall-tangential projection:

$$\mathbf{P}_S = \mathbf{I} - \vec{n}_S \otimes \vec{n}_S$$

No-penetration condition: $\vec{u} \cdot \vec{n}_S = 0$ on $\partial\Omega_S$

Effective wall force: $$\mu \mathbf{P}_S (\nabla \vec{u} + \nabla \vec{u}^T) \vec{n}_S = \underbrace{-\beta_S \mathbf{P}_S \vec{u}}_{=\vec{f}_{S,\text{diss}}(\vec{u})} \quad \text{on } \partial\Omega_S$$

Contact line force: $$\beta_L (\vec{u} \cdot \vec{n}_L) \vec{n}_L = \sigma \left(\cos(\theta_{stat}) - \cos(\theta)\right) \vec{n}_L \quad \text{on } L$$

# EXTENDED DISCONTINUOUS GALERKIN DISCRETIZATION

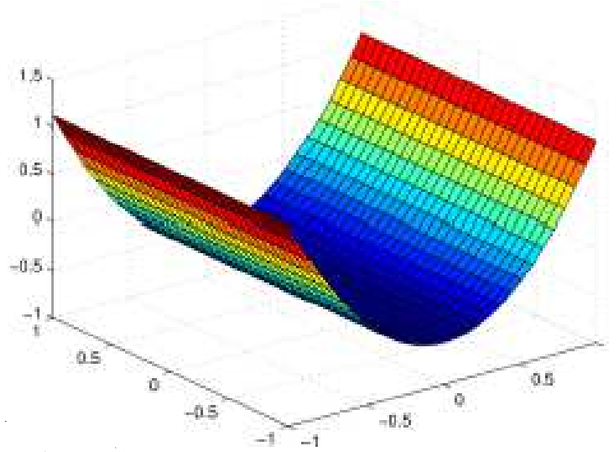
TECHNISCHE UNIVERSITÄT DARMSTADT

# BASIC IDEA: EXTENDED DISCONTINUOUS GALERKIN

TECHNISCHE UNIVERSITÄT DARMSTADT

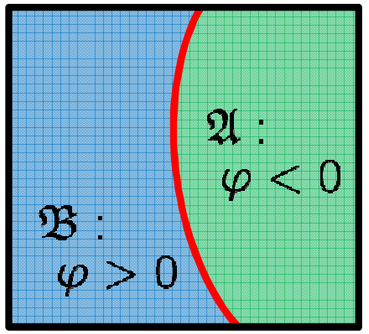
Approximation of $u(\vec{x}, t)$:
(in each cell $K_j$)

$$u_j(\vec{x}, t) = \sum_{n=1}^{N} \tilde{u}_{j,n}(t)\Phi_{j,n}(\vec{x})$$

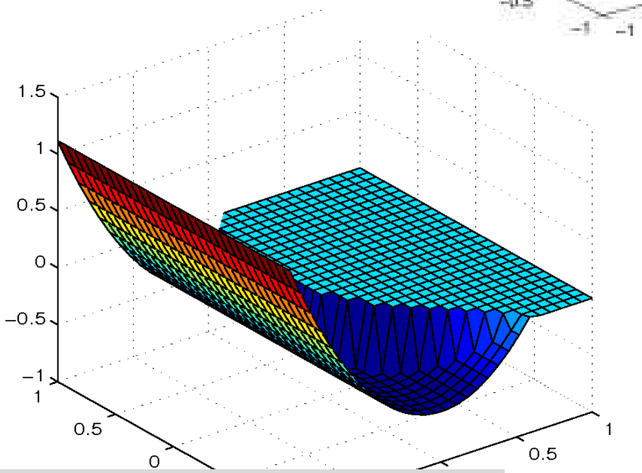


$\Phi_4(\boldsymbol{x})$

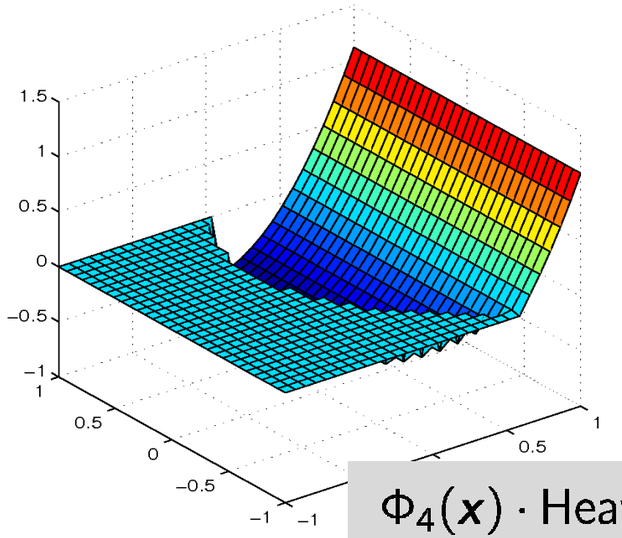
Approximation of
Interface $\mathfrak{I}$:
Level-Set function $\varphi$




$\mathfrak{I} : \varphi = 0$

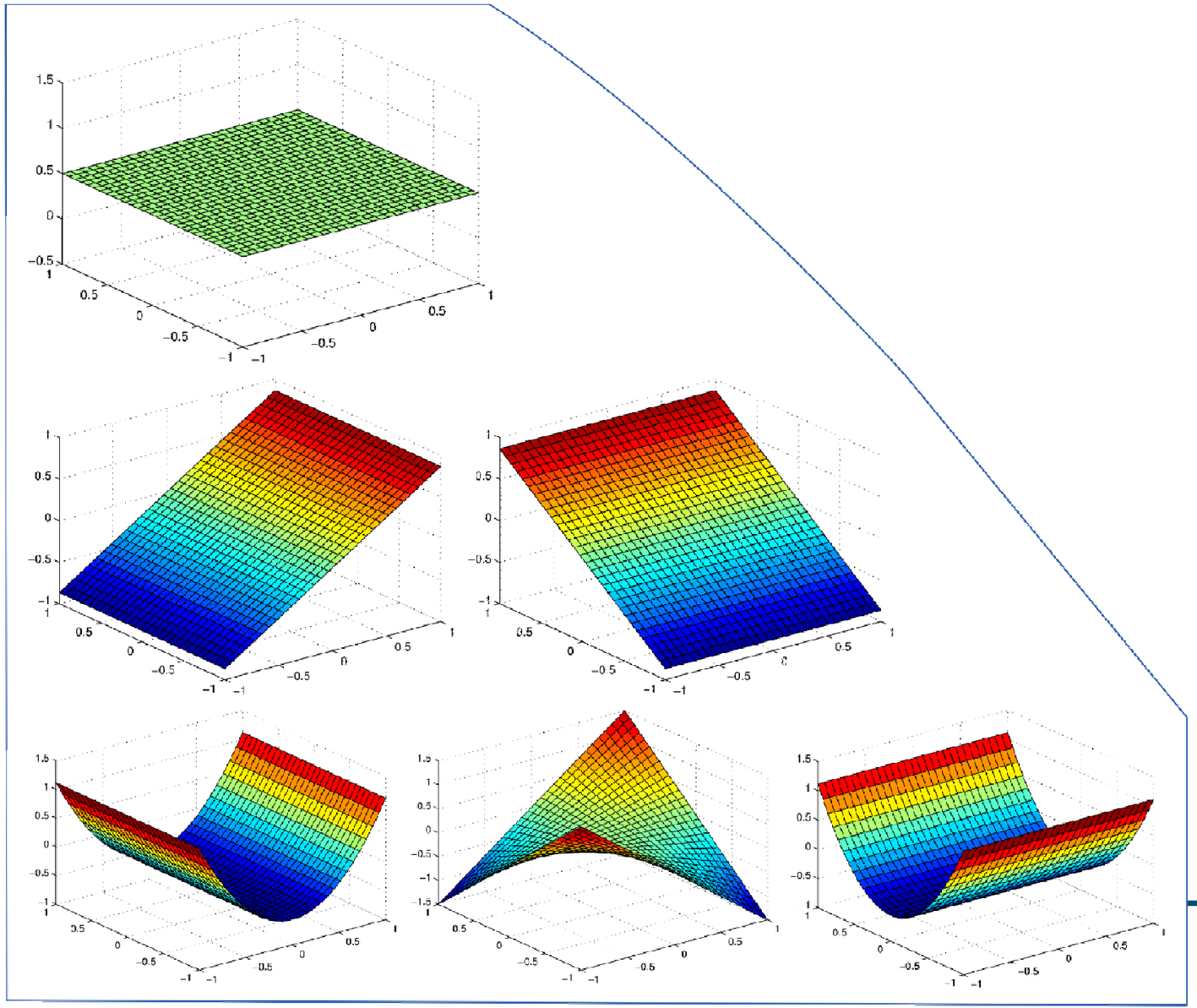


$\Phi_4(\boldsymbol{x}) \cdot \text{Heaviside}(+\varphi(\boldsymbol{x}))$



$\Phi_4(\boldsymbol{x}) \cdot \text{Heaviside}(-\varphi(\boldsymbol{x}))$

# FROM DG…



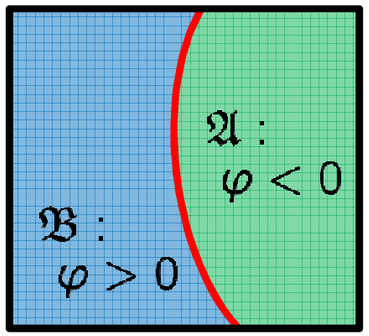
Polynomial degree 2,
spatial dimension 2

$$u_j(\vec{x}, t) = \sum_{n=1}^{N} \tilde{u}_{j,n}(t)\Phi_{j,n}(\vec{x})$$

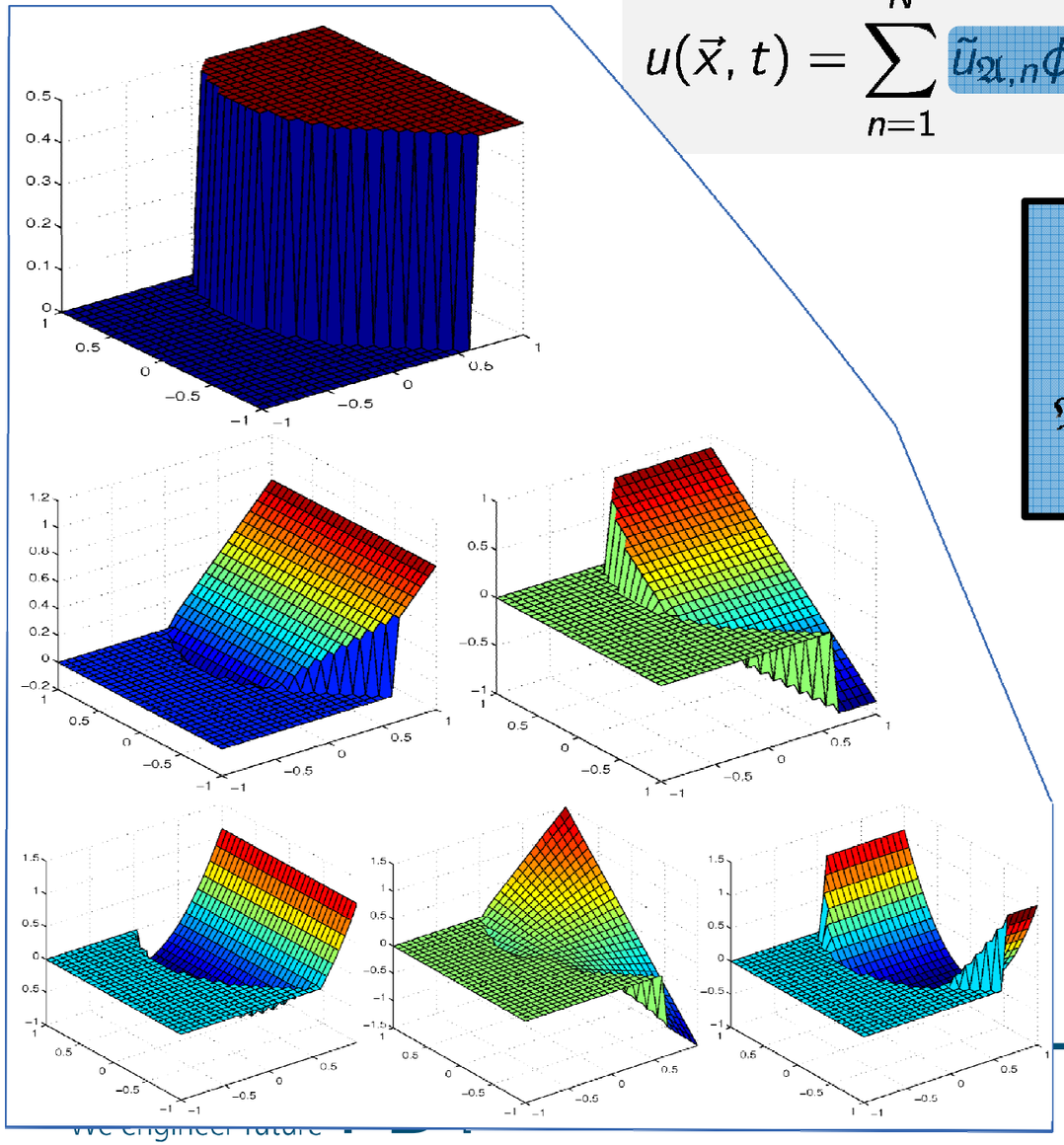
# … TO XDG

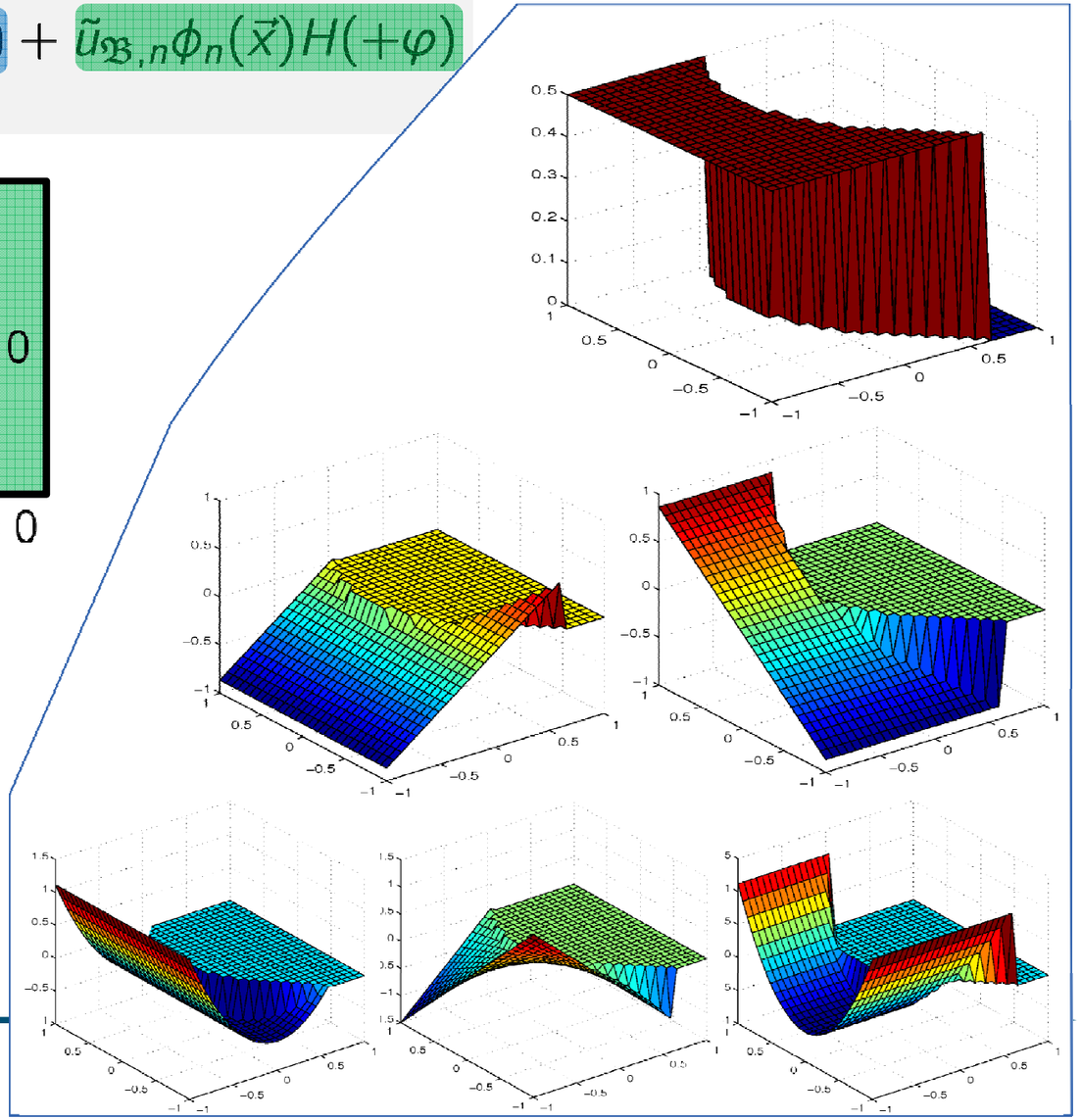
TECHNISCHE UNIVERSITÄT DARMSTADT

$$u(\vec{x},t) = \sum_{n=1}^{N} \tilde{u}_{\mathfrak{A},n}\phi_n(\vec{x})H(-\varphi) + \tilde{u}_{\mathfrak{B},n}\phi_n(\vec{x})H(+\varphi)$$




$\mathfrak{I} : \varphi = 0$





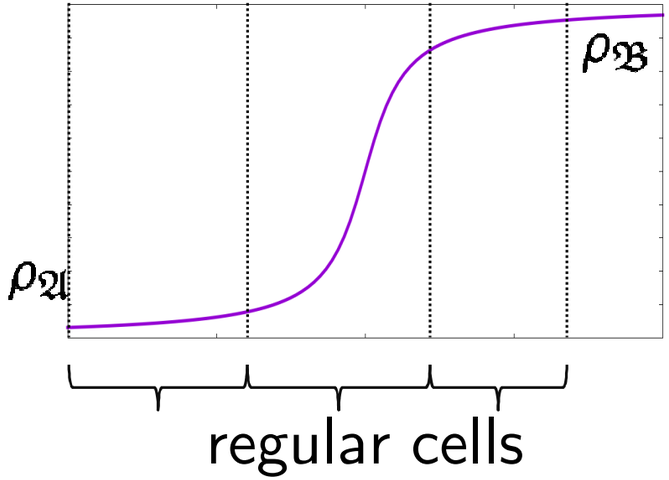
# REMARK: SHARP VS. SMOOTH INTERFACE

TECHNISCHE UNIVERSITÄT DARMSTADT

- Smooth interface (artificially thickened):
  - no adaption of approximation space

$$\text{e.g. } \rho = a + \tan^{-1}(\varphi) b$$

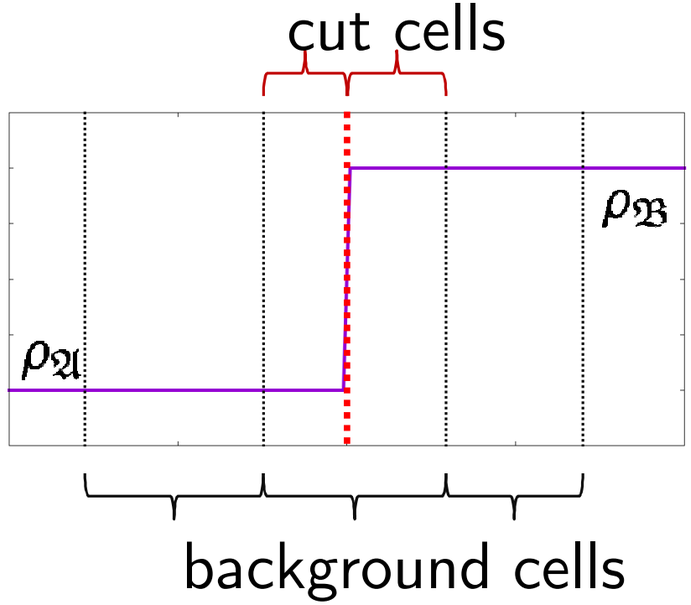
  - mass conservation: “easy”, low accuracy: solving a regularized problem




- **Sharp interface: XDG**

$$\rho = \rho_{\mathfrak{A}} + \text{Heaviside}(\varphi)(\rho_{\mathfrak{B}} - \rho_{\mathfrak{A}})$$

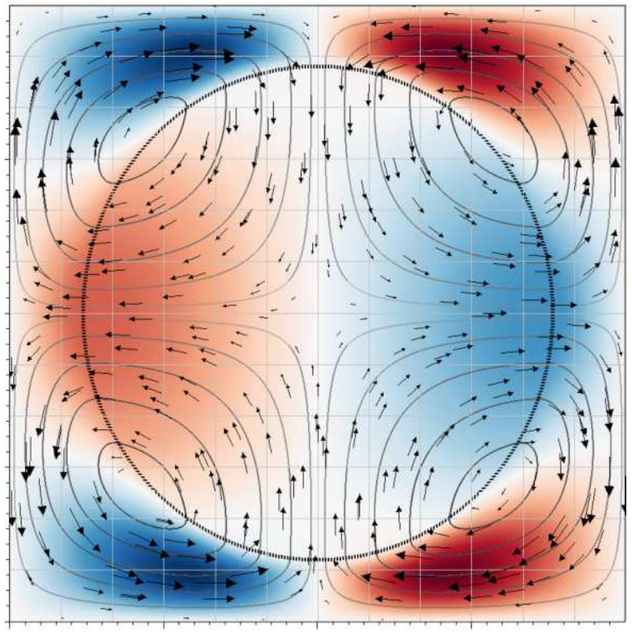
  - cut-cells: approx. space is adapted to problem
  - jumps are infinitely sharp, can appear within a background cell
  - high accuracy, mass conservation difficult

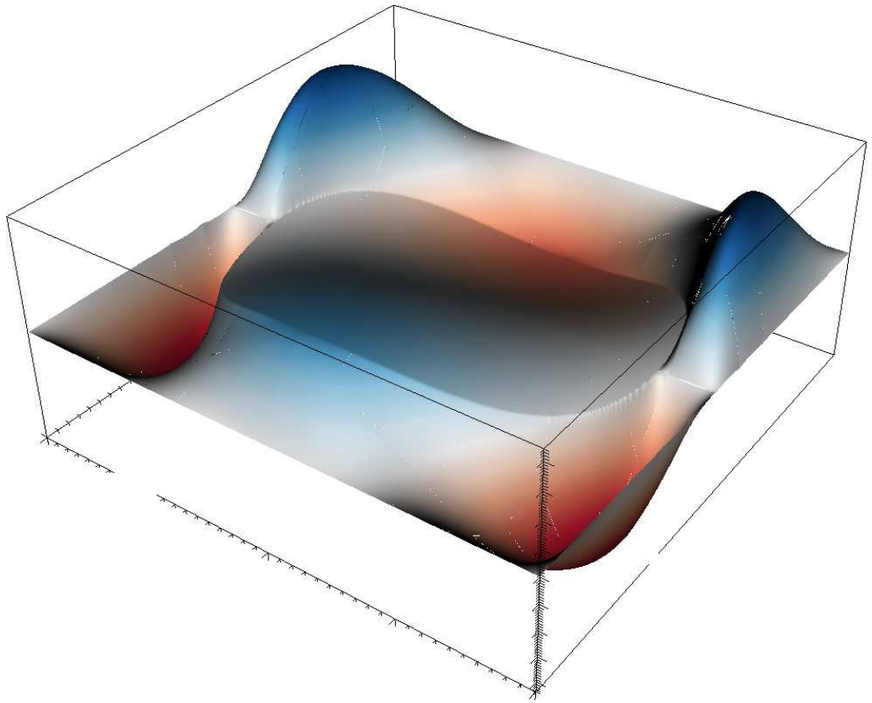


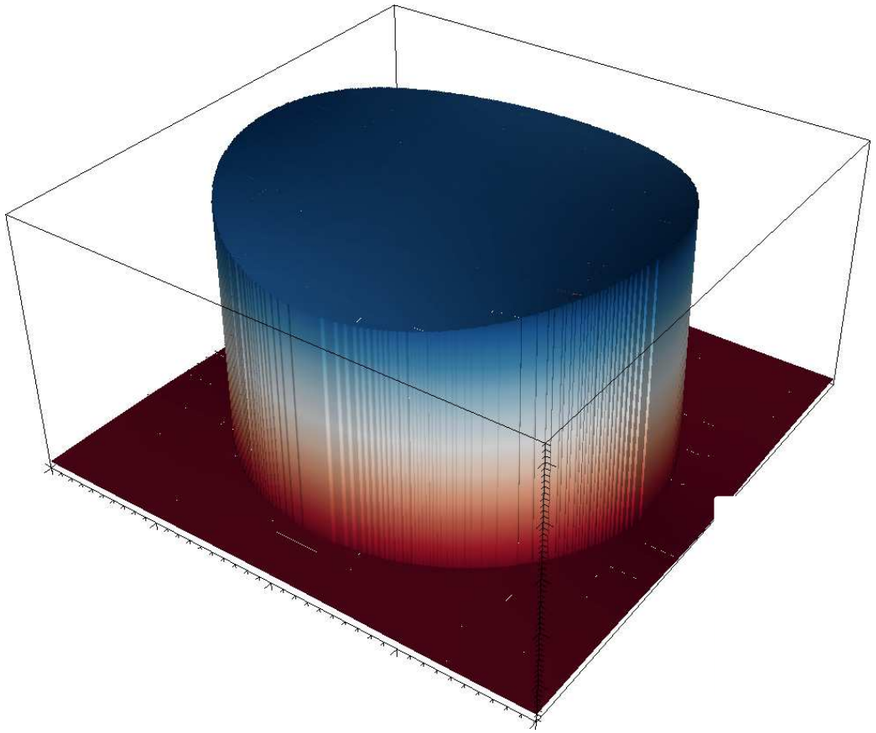
# SHARP INTERFACE METHODS

TECHNISCHE UNIVERSITÄT DARMSTADT

- Oscillating Droplet: water/air; 10 cells across Droplet
- Sharp representation of velocity kink and pressure jump



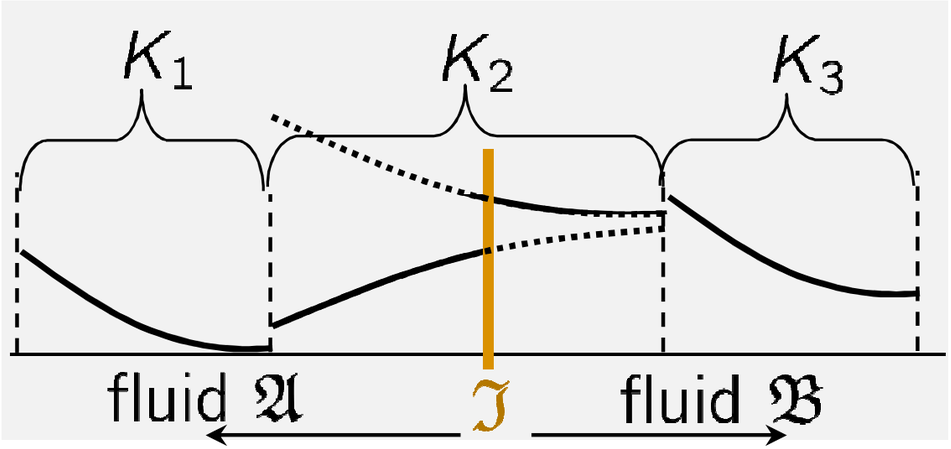




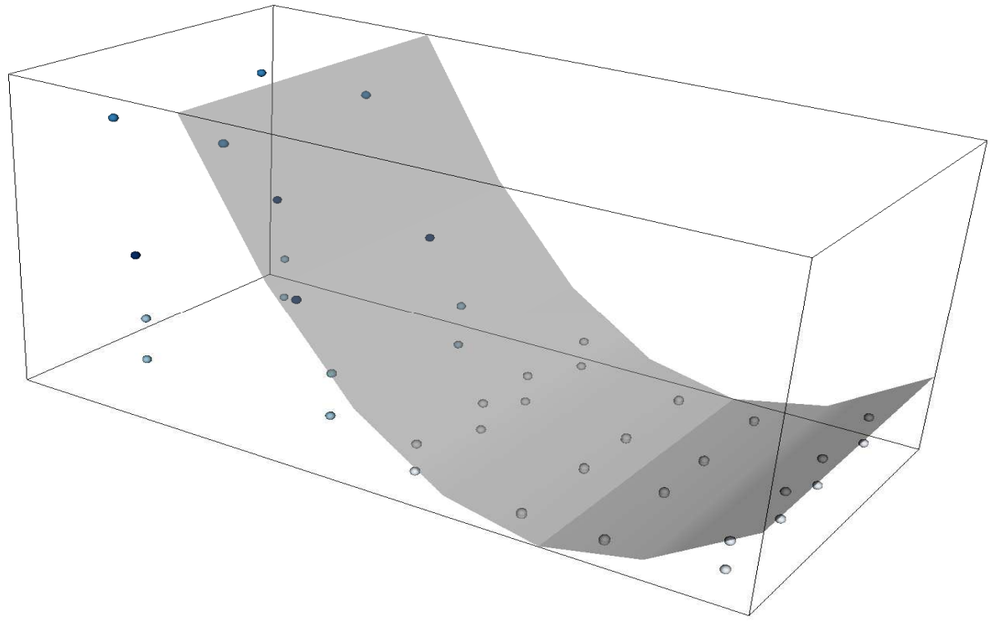
# IMPLEMENTATION

TECHNISCHE UNIVERSITÄT DARMSTADT

- Store a second set of DOF's in cut-cells, i.e. use dynamic data structures
- Agglomeration of very small cut-cells

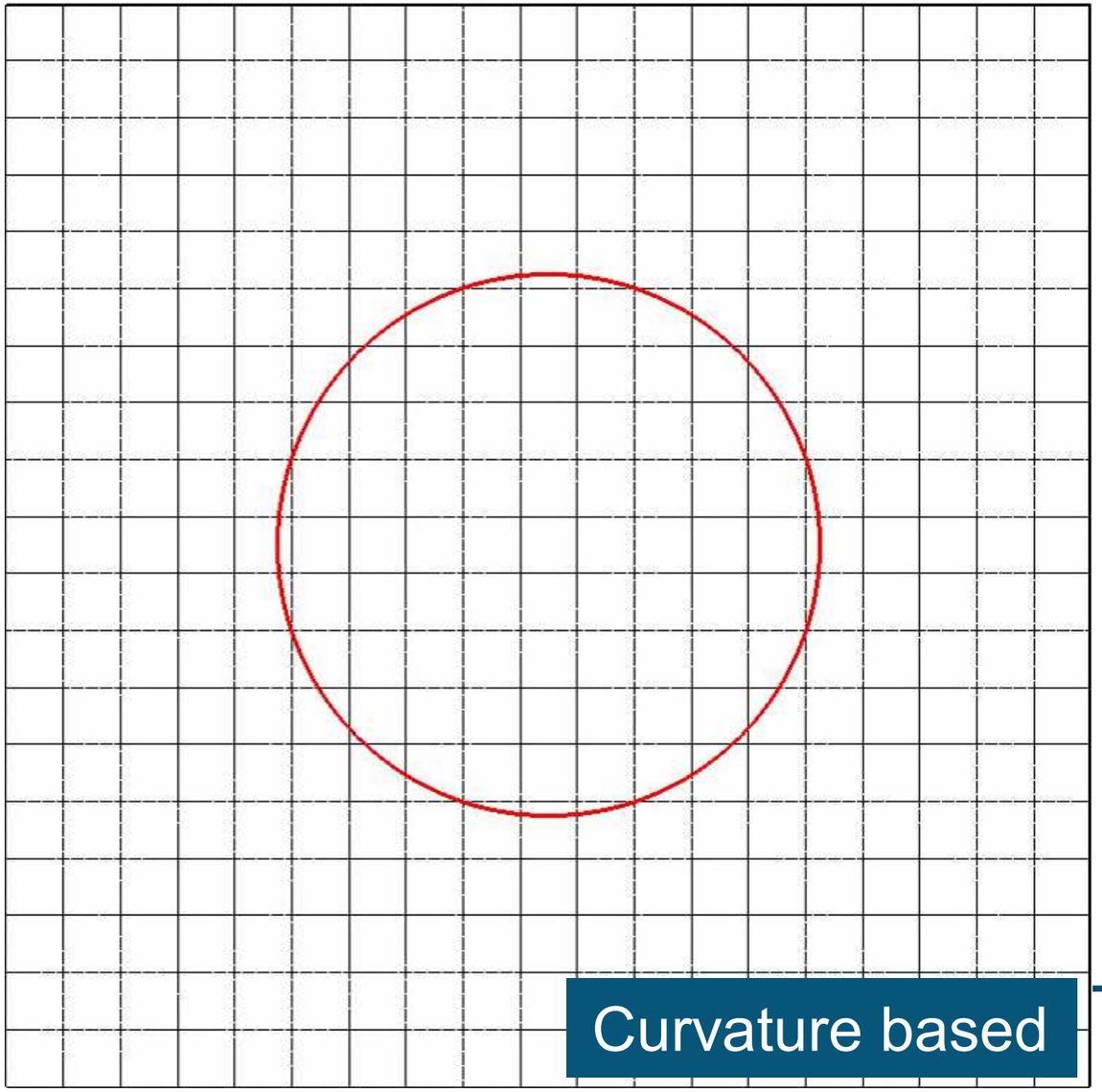



- construct quadrature rules for cut cells
  - libraries available: e.g. Müller & Kummer, Saye, Fries, Ventura

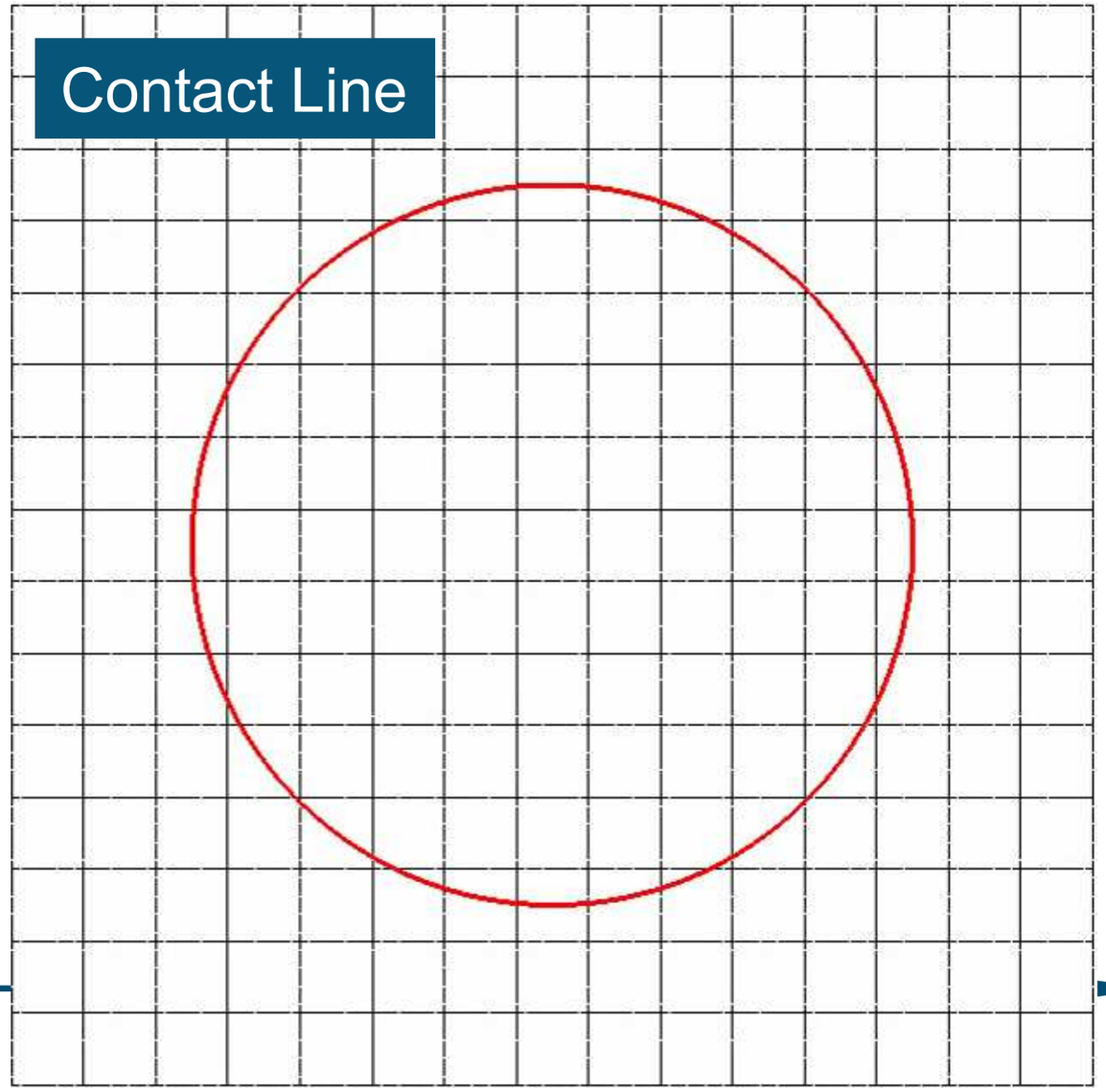


# FEATURE-BASED ADAPTIVE REFINEMENT

TECHNISCHE UNIVERSITÄT DARMSTADT

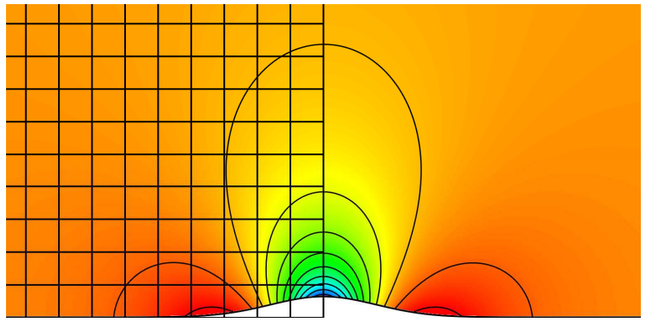


Curvature based



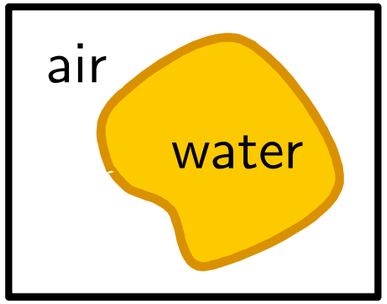
Contact Line

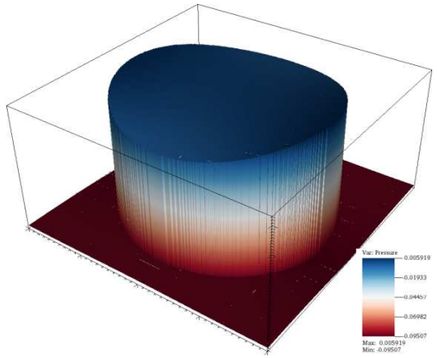
# OTHER XDG APPLICATIONS

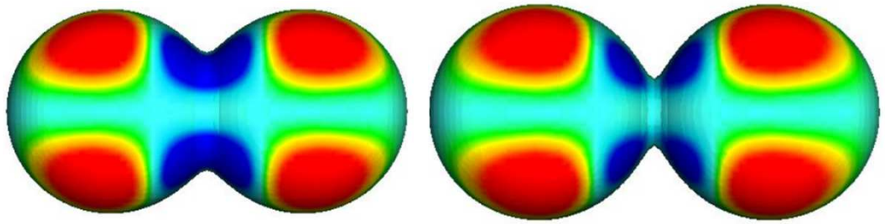


Immersed boundary methods
(Compressible /
Incompressible)

Multiphase flows
(jumps in pressure and
velocity gradient)

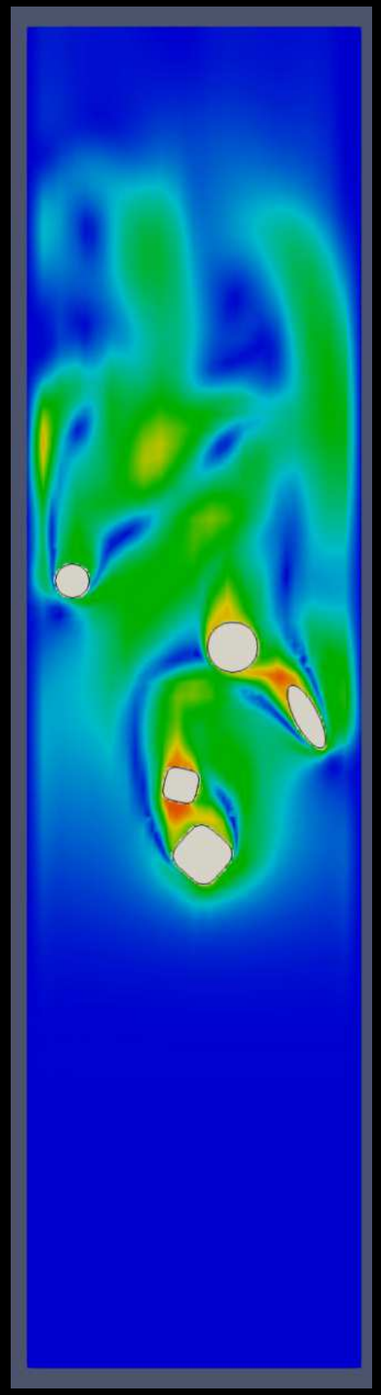


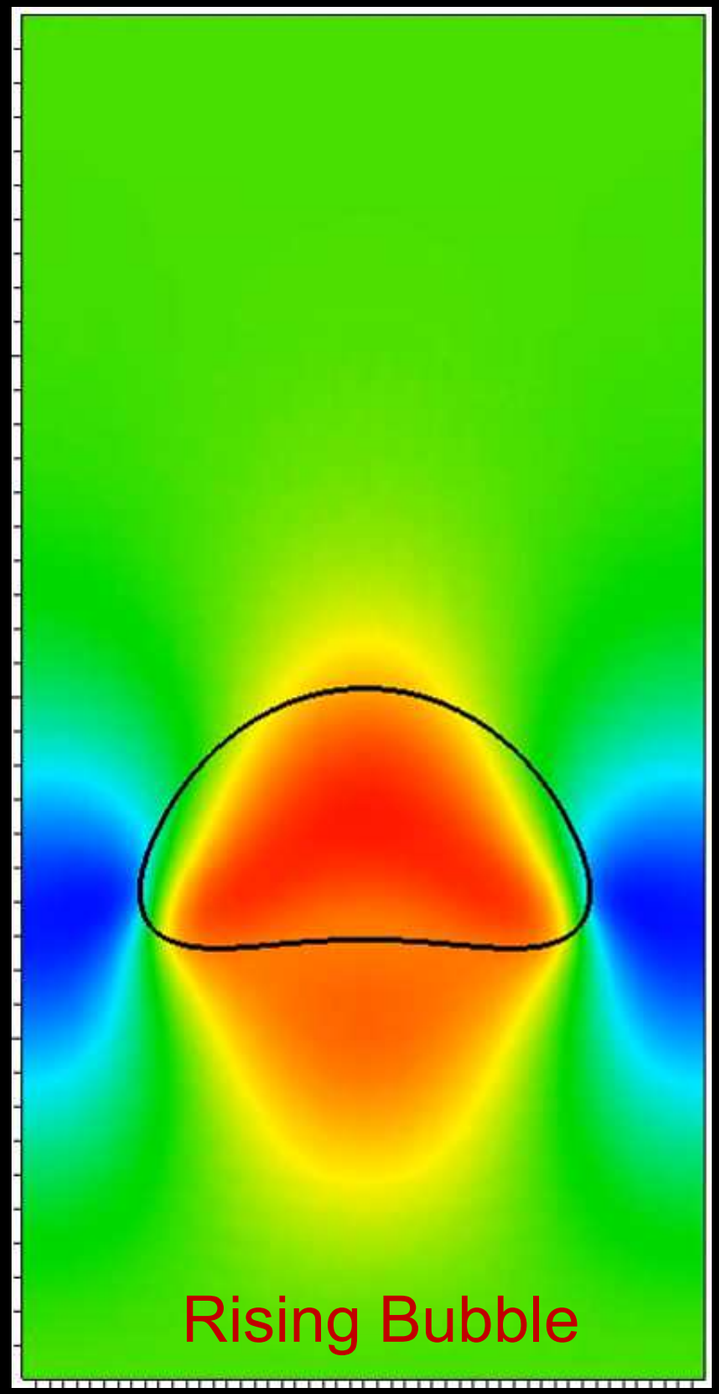


Interfacial equations
(surfactant transport)

# OTHER XDG SIMULATIONS



Particle System



Rising Bubble

# NUMERICAL METHOD

TECHNISCHE UNIVERSITÄT DARMSTADT

# WEAK FORM (TWO PHASE)

TECHNISCHE UNIVERSITÄT DARMSTADT

In the XDG-space, solve the variational problem

$$(\partial_t(\rho\vec{u}),\vec{v}) + t(\vec{u},\vec{u},\vec{v}) + b(p,\vec{v}) + a(\vec{u},\vec{v}) = \oint_{\mathfrak{I}} \sigma\kappa\vec{n}_{\mathfrak{I}} \cdot [\![\vec{v}]\!] \, \mathrm{dS} + \mathrm{bc}(\vec{v})$$

$$b(\tau,\vec{u}) = 0$$

viscous:

$$a(\vec{u},\vec{v}) = -\int_\Omega \mu(\nabla_h\vec{u} : \nabla_h\vec{v} + (\nabla_h\vec{u})^T : \nabla_h\vec{v})\mathrm{dV} \quad \text{SIP}$$
$$+ \oint_{(\Gamma\setminus\Gamma_N)\cup\mathfrak{I}} \left(\{\{\mu\left(\nabla_h\vec{u} + \nabla_h\vec{u}^T\right)\}\}\,\vec{n}_{\mathfrak{I},\Gamma}\right)\cdot[\![\vec{v}]\!] + \left(\{\{\mu\left(\nabla_h\vec{v} + \nabla_h\vec{v}^T\right)\}\}\,\vec{n}_{\mathfrak{I},\Gamma}\right)\cdot[\![\vec{u}]\!]\mathrm{dS}$$
$$- \oint_{(\Gamma\setminus\Gamma_N)\cup\mathfrak{I}} \eta[\![\vec{u}]\!]\cdot[\![\vec{v}]\!]\mathrm{dS}.$$

convection:

$$t(\vec{w},\vec{u},\vec{v}) = -\int_\Omega \rho(\vec{u}\otimes\vec{w}) : \nabla_h\vec{v}\mathrm{dV} - \oint_{\Gamma_{\mathrm{int}}\cup\Gamma_N\cup\mathfrak{I}} \left(\{\{\vec{u}\otimes\vec{w}\}\}\,\vec{n}_{\mathfrak{I},\Gamma} + (\lambda/2)[\![\vec{u}]\!]\right)\cdot[\![\rho\vec{v}]\!]\mathrm{dS} \quad \text{LLF}$$

pressure grad./
velocity div.:

$$b(p,\vec{v}) = -\int_\Omega p\ \mathrm{div}_h\left(\vec{v}\right)\mathrm{dV} - \oint_{(\Gamma\setminus\Gamma_N)\cup\mathfrak{I}} [\![\vec{v}]\!]\cdot\vec{n}_{\mathfrak{I},\Gamma}\,\{\{p\}\}\,\mathrm{dS}$$

INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
*Int. J. Numer. Meth. Engng* (2016)
Published online in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/nme.5288

# Extended discontinuous Galerkin methods for two-phase flows: the spatial discretization

Florian Kummer[1,2,*,†]

[1] *Fluid Dynamics, Technische Universität Darmstadt, Otto-Berndt-Str. 2, D-64287 Darmstadt, Germany*
[2] *Graduate School Computational Engineering, Technische Universität Darmstadt, Dolivostr. 15, D-64293 Darmstadt, Germany*

## SUMMARY

This work discusses a discontinuous Galerkin (DG) discretization for two-phase flows. The fluid interface is represented by a level set, and the DG approximation space is adapted such that jumps and kinks in pressure and velocity fields can be approximated sharply. This adaption of the original DG space, which can be performed 'on-the-fly' for arbitrary interface shapes, is referred to as extended discontinuous Galerkin.

We engineer future

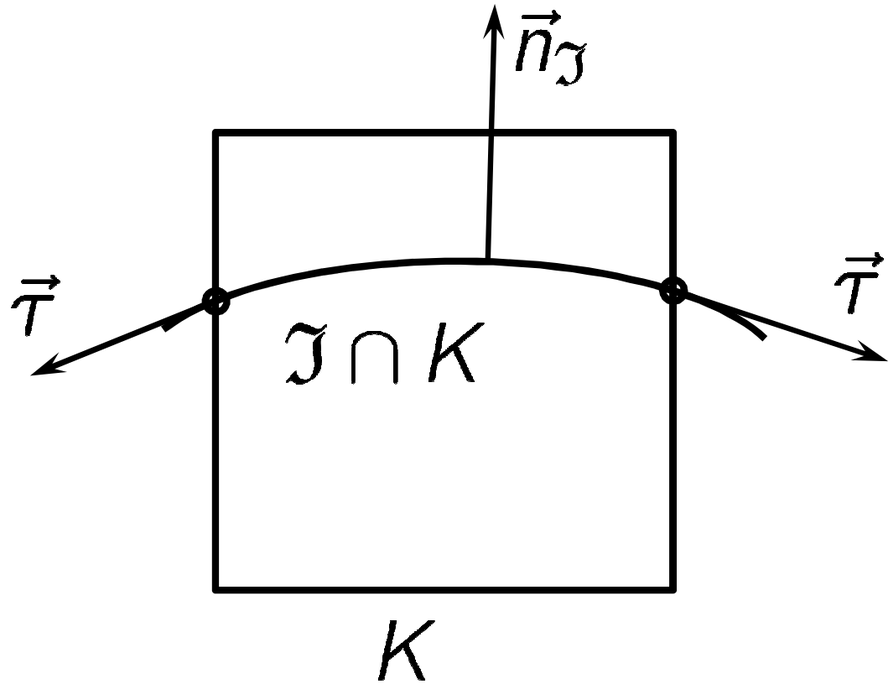
# SURFACE TENSION

TECHNISCHE UNIVERSITÄT DARMSTADT

- Curvature-based (2nd deriv.) vs. Tension-based (1st deriv.)

$$\oint_{\mathfrak{I}\cap K} \kappa \vec{n}_{\mathfrak{I}} \, \mathrm{dS} \, \mathrm{dS} = -\oint_{\mathfrak{I}\cap \partial K} \vec{\tau} \, \mathrm{d}\ell$$

$$\kappa = \mathrm{div}(\vec{n}_{\mathfrak{I}}) = \mathrm{div}\left(\frac{\nabla\varphi}{\|\nabla\varphi\|}\right)$$




- „High Order“: Stokes theorem:

$$\oint_{\mathfrak{I}\cap K} \kappa \vec{n}_{\mathfrak{I}} \cdot \vec{v} \, \mathrm{dS} \, \mathrm{dS} = \oint_{\mathfrak{I}\cap K} (\mathbf{I} - \vec{n}_{\mathfrak{I}} \otimes \vec{n}_{\mathfrak{I}}) : \nabla \vec{v} \, \mathrm{dS} - \oint_{\mathfrak{I}\cap \partial K} \vec{\tau} \cdot \vec{v} \, \mathrm{d}\ell$$

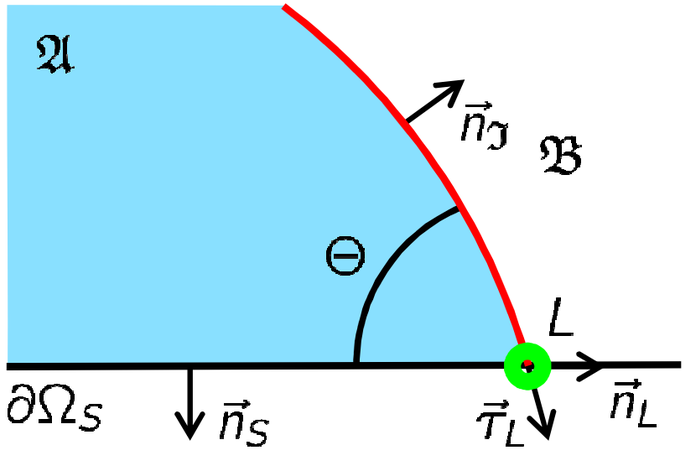
# WEAK FORM, EXTENSION FOR CONTACT LINE

TECHNISCHE UNIVERSITÄT DARMSTADT

2-Phase:

$$(\partial_t(\rho\vec{u}),\vec{v}) + \underbrace{CPV(\vec{u},\vec{u},p,\vec{v})}_{\text{conv, pressure \& viscous}} = \mathrm{bc}(\vec{v})$$

$$+ \oint_{\mathfrak{I}} \sigma\kappa\vec{n}_{\mathfrak{I}} \cdot [\![\vec{v}]\!] \; \mathrm{dS}$$




2-Phase

plus

3-Phase contact line:

$$(\partial_t(\rho\vec{u}),\vec{v}) + \underbrace{CPV(\vec{u},\vec{u},p,\vec{v})}_{\text{conv, pressure \& viscous}} = \mathrm{bc}(\vec{u},\vec{v})$$

$$+ \oint_{\mathfrak{I}} \sigma(\mathbf{I} - \vec{n}_{\mathfrak{I}} \otimes \vec{n}_{\mathfrak{I}}) : [\![\nabla\vec{v}]\!] \; \mathrm{dS} - \int_{\mathfrak{I}\cap\Gamma_i} \sigma \{\{\vec{\tau}\}\} \cdot [\![\vec{v}]\!] \; \mathrm{d}\ell$$

$$+ \int_L (\beta_L(\vec{u}\cdot\vec{n}_L)\vec{n}_L - \sigma(\cos(\theta_{stat}) - \cos(\theta))\,\vec{n}_L) \cdot [\![\vec{v}]\!] \; \mathrm{d}\ell$$

# RESULTS

TECHNISCHE UNIVERSITÄT DARMSTADT

MASCHINENBAU
We engineer future FDY

# SLIDING DROPLET TO EQUILIBRIUM STATE

TECHNISCHE UNIVERSITÄT DARMSTADT

Initial Contact Angle $\theta_0 = 90°$

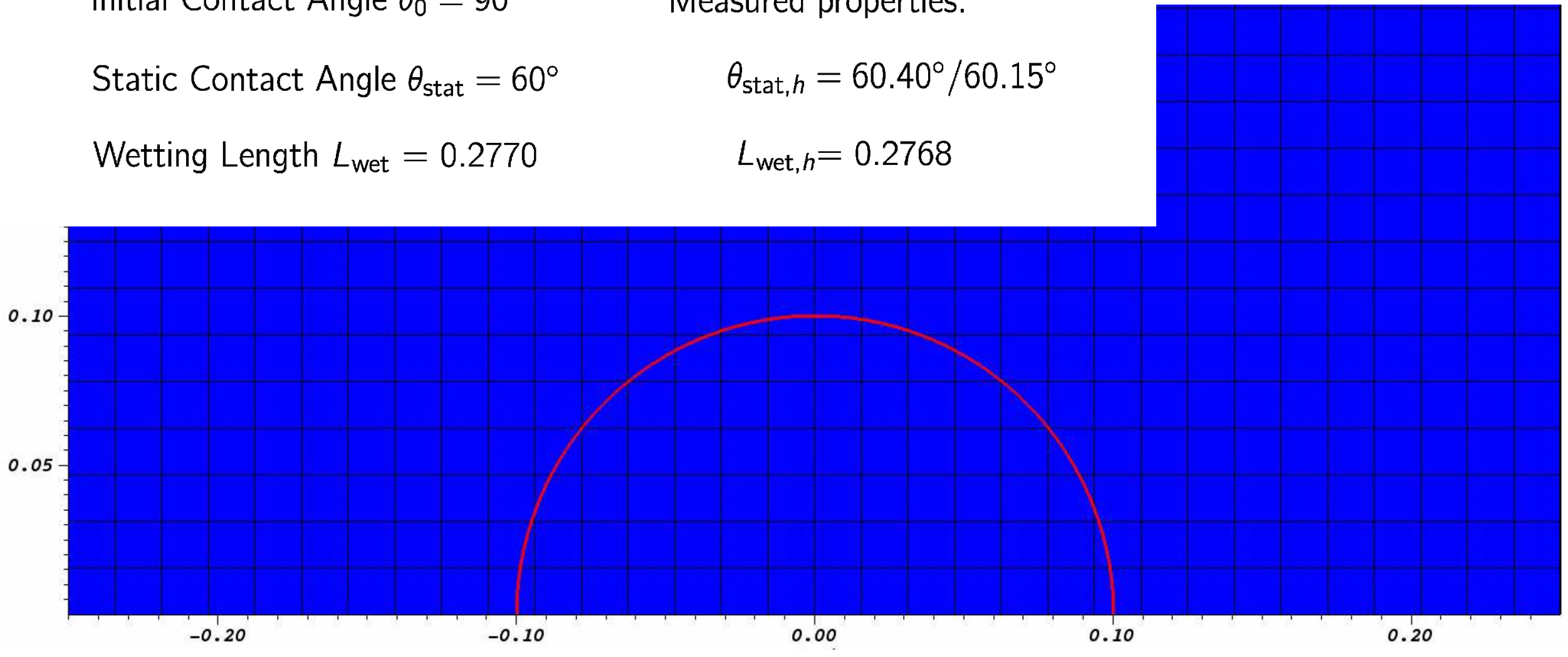
Static Contact Angle $\theta_{stat} = 60°$

Wetting Length $L_{wet} = 0.2770$

Measured properties:

$\theta_{stat,h} = 60.40°/60.15°$

$L_{wet,h} = 0.2768$



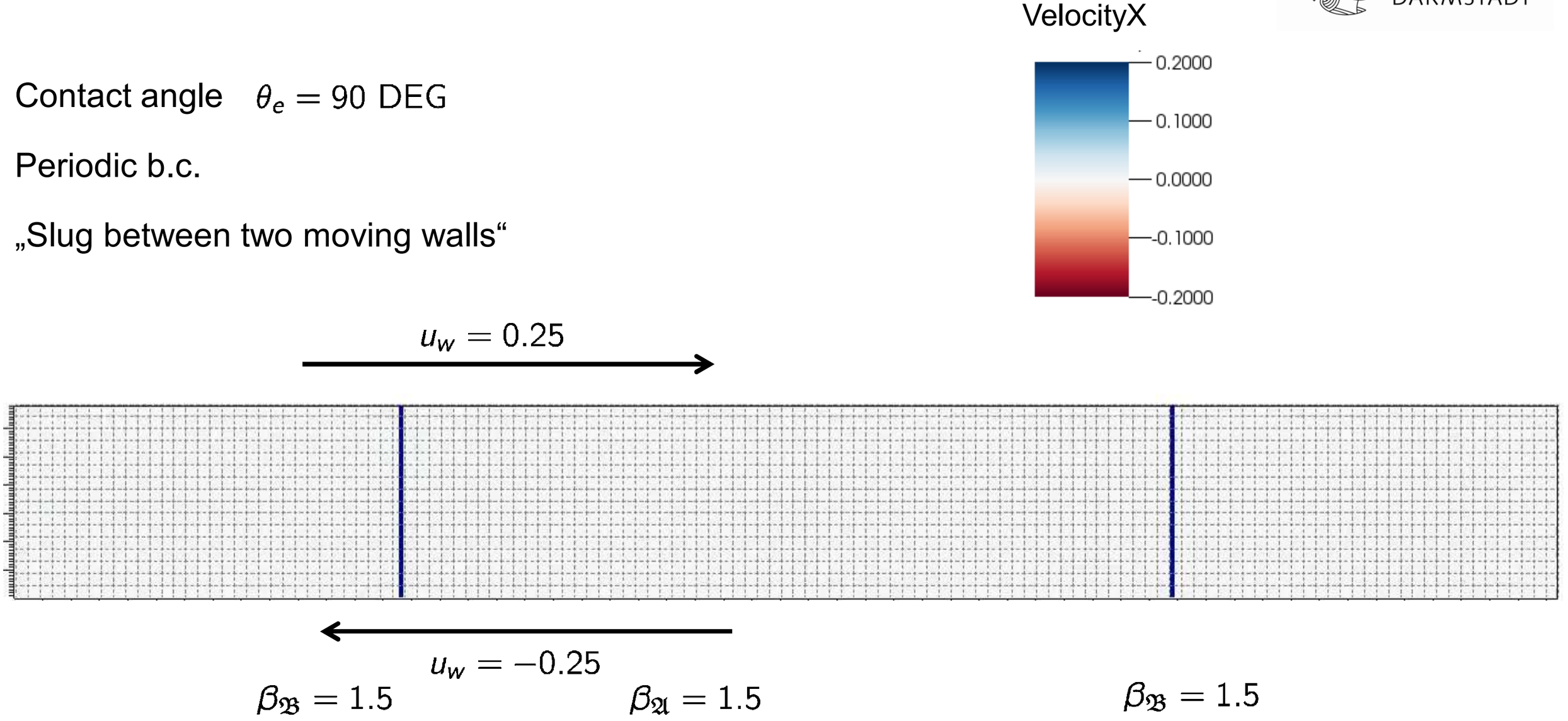
# SYMMETRIC CHANNEL

TECHNISCHE UNIVERSITÄT DARMSTADT

Contact angle $\theta_e = 90$ DEG

Periodic b.c.

„Slug between two moving walls“



# GNBC IN 3D

TECHNISCHE UNIVERSITÄT DARMSTADT

Static droplet on a plate:

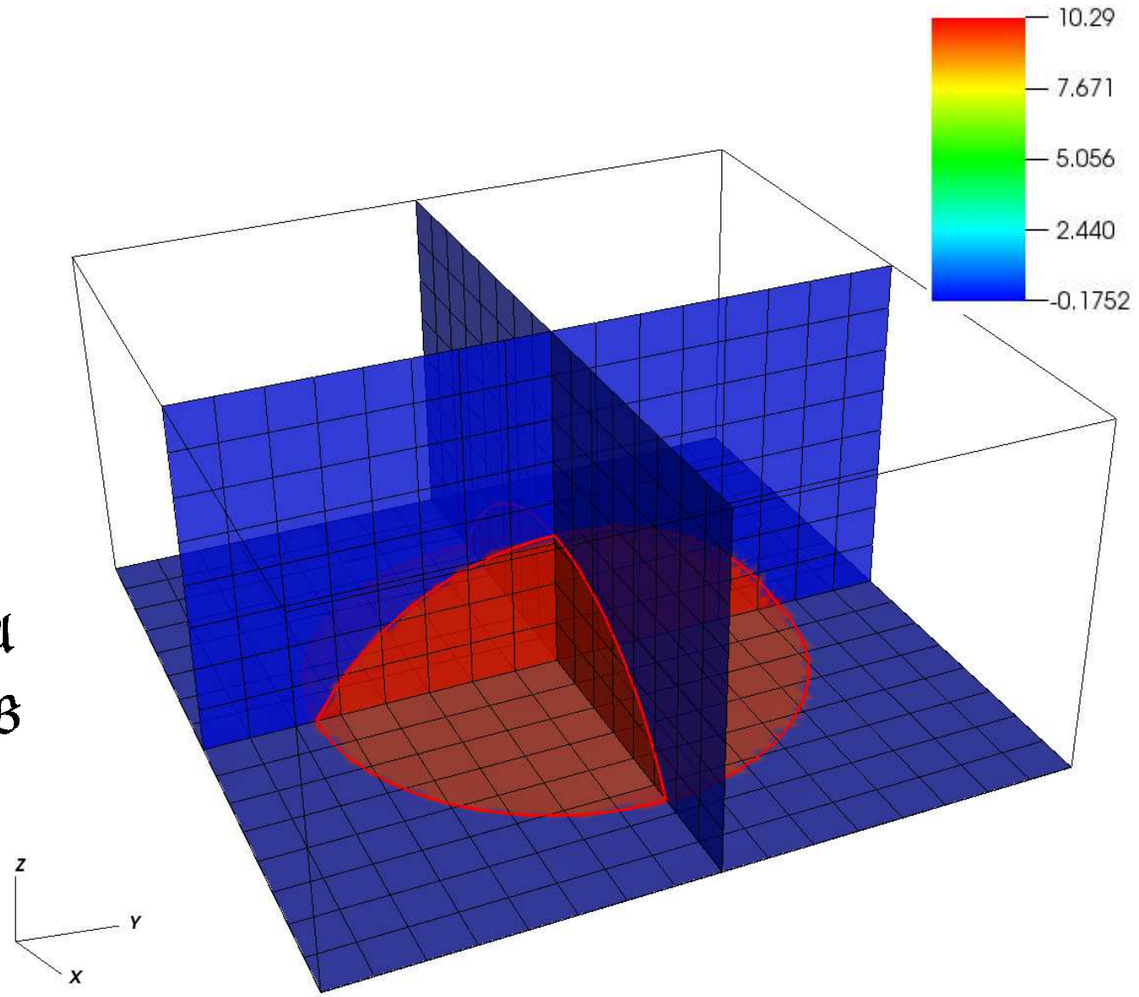
$$\theta = \theta_e = 60°$$

$$R = 0.1$$

$$\sigma = 0.5$$

$$p_{\text{steady}} = \begin{cases} p_0 + p_{\text{jump}} & \text{in } \mathfrak{A} \\ p_0 & \text{in } \mathfrak{B} \end{cases}$$

$$p_{\text{jump}} = \frac{2\sigma}{R} = 10$$

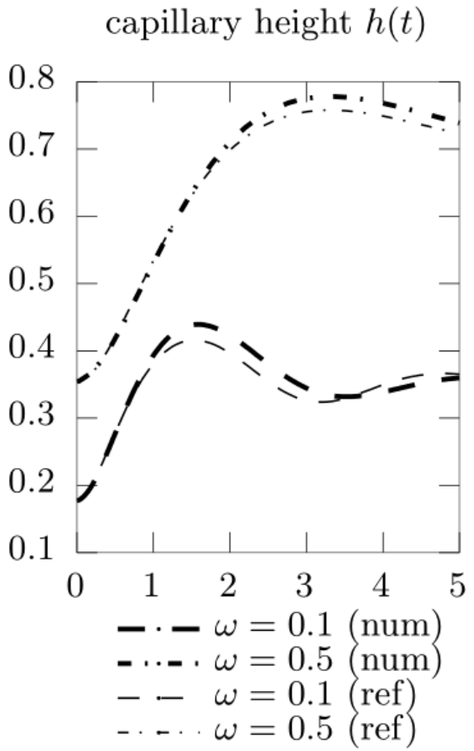


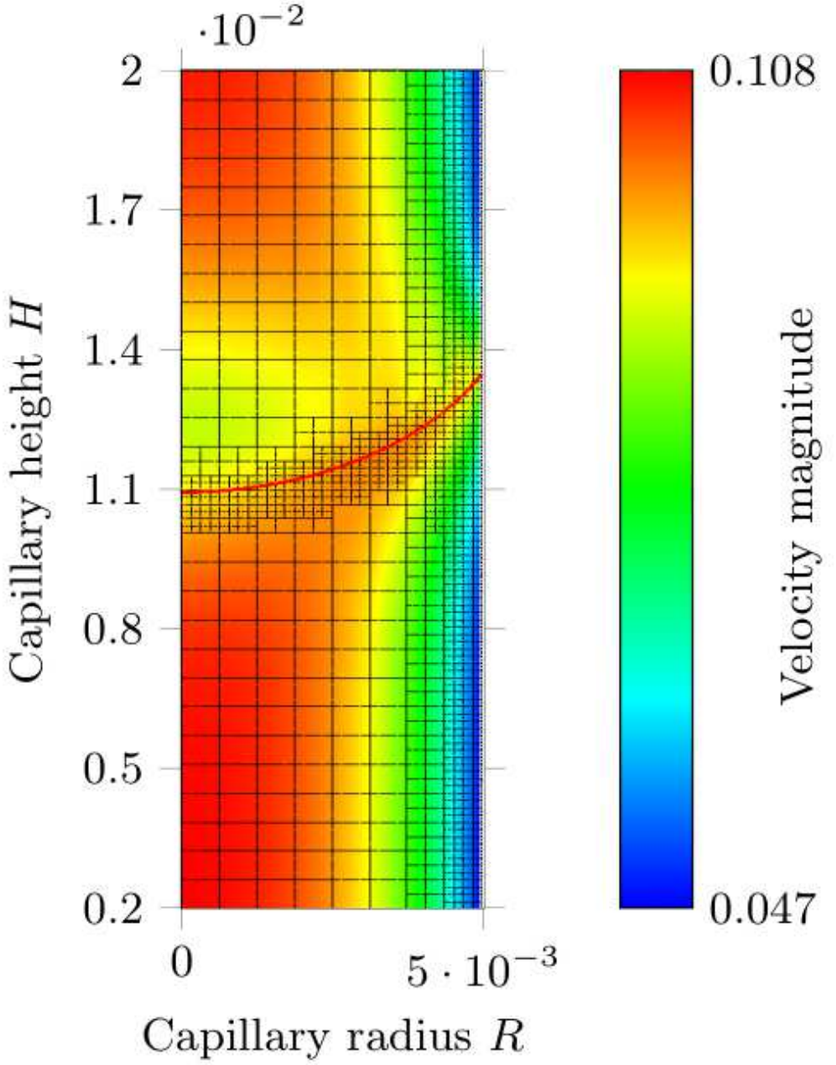
# VALIDATION: CAPILLARY RISE

- Fluid rising in a small diameter tube (capillary)
- Comparison against semi-analytical solution for rise height over time

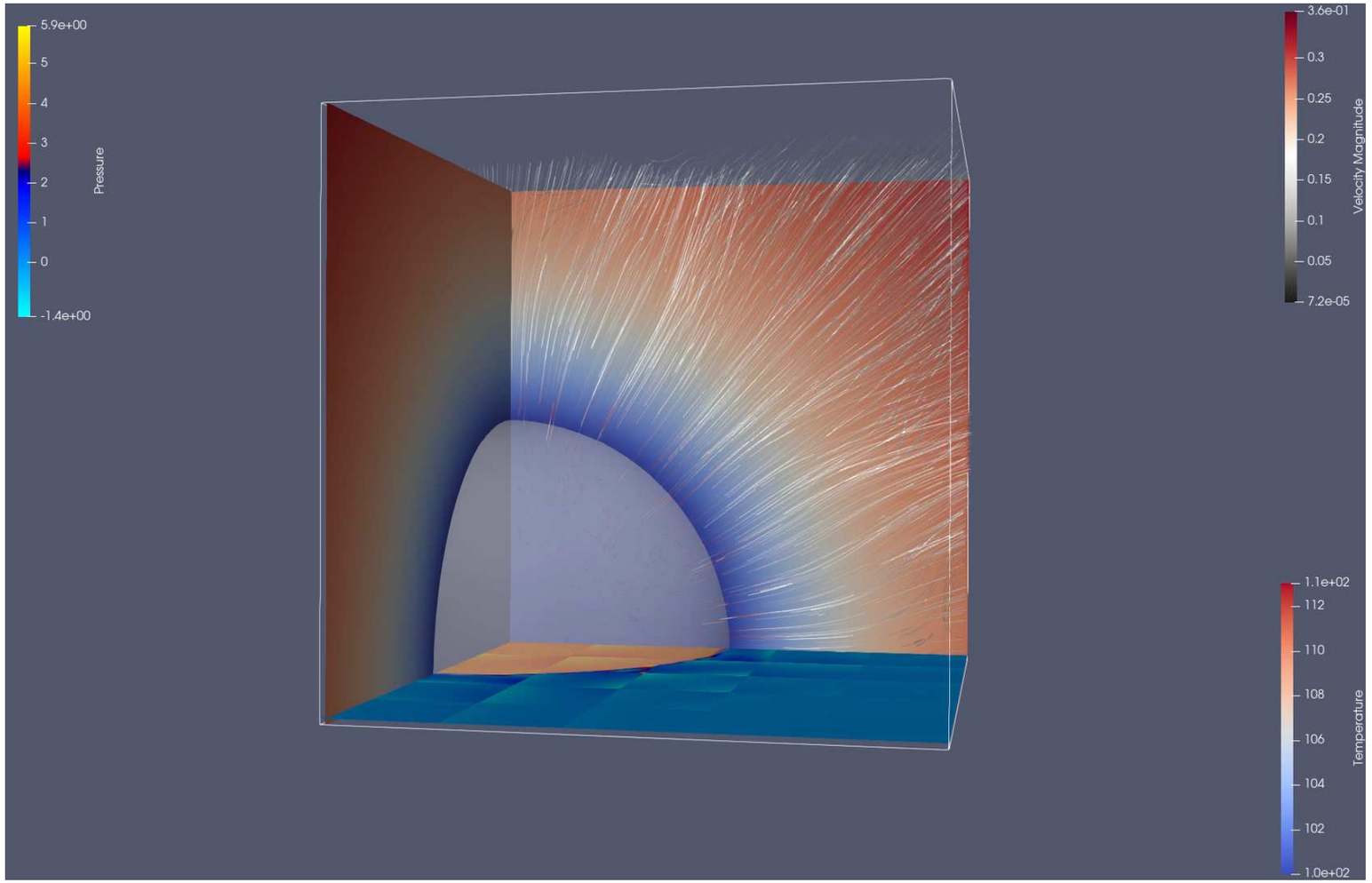
Comparison of different codes within SFB1194

$$\omega := \sqrt{\frac{9\sigma \cos(\theta_{stat})\mu^2}{\rho^3 g^2 R^5}}$$



# DROPLET EVAPORATION



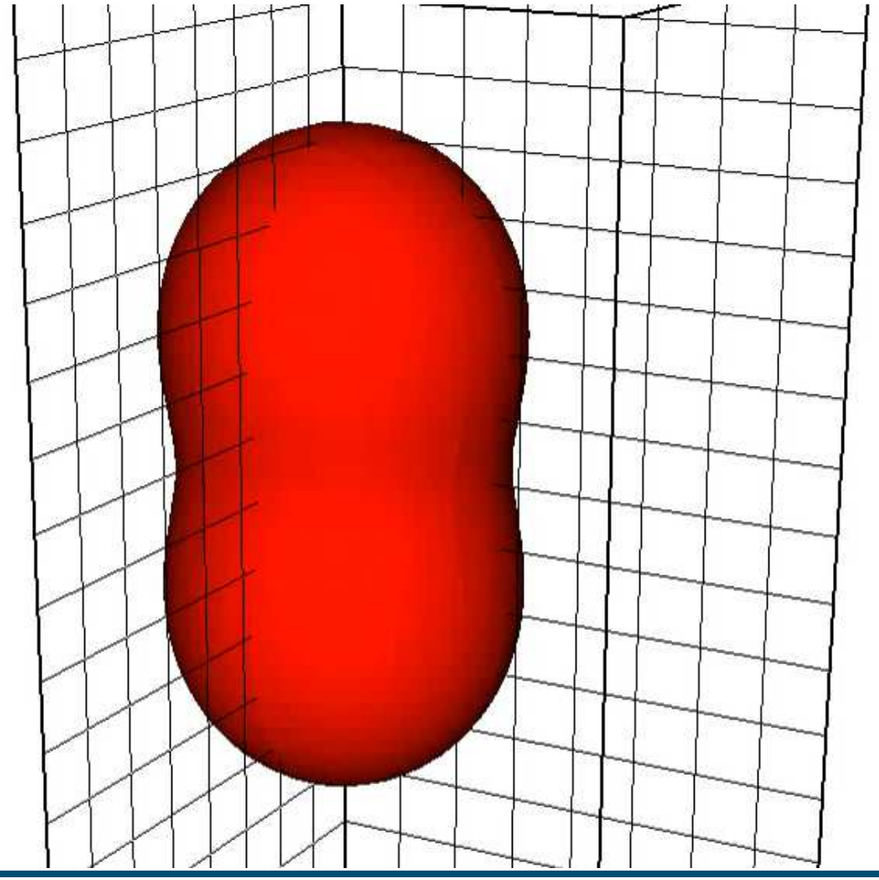

## HIGHLIGHTS & FEATURES:

- High density and viscosity ratios.
- Mass transfer across interface
- Heat transfer across interface
- Dynamic contact line (droplet sitting on solid surface)

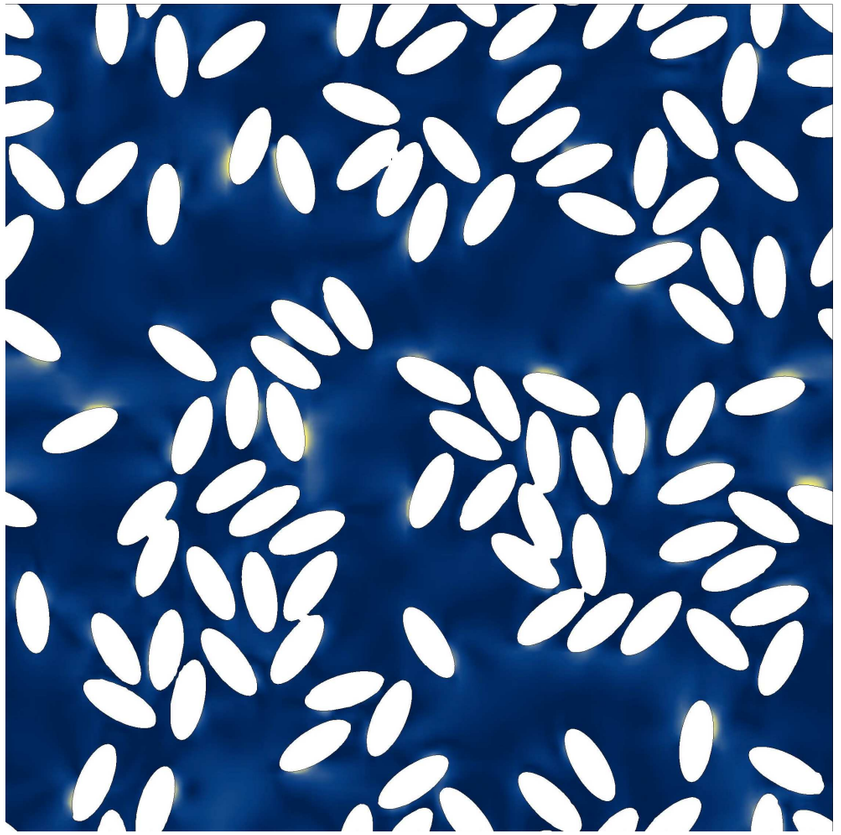
# FURTHER DEMONSTRATIONS

TECHNISCHE UNIVERSITÄT DARMSTADT

## DROPLET OSCILLATION



## ACTIVE SWIMMERS (BACTERIA)



# SUMMARY & OUTLOOK (PART 2)

TECHNISCHE UNIVERSITÄT DARMSTADT

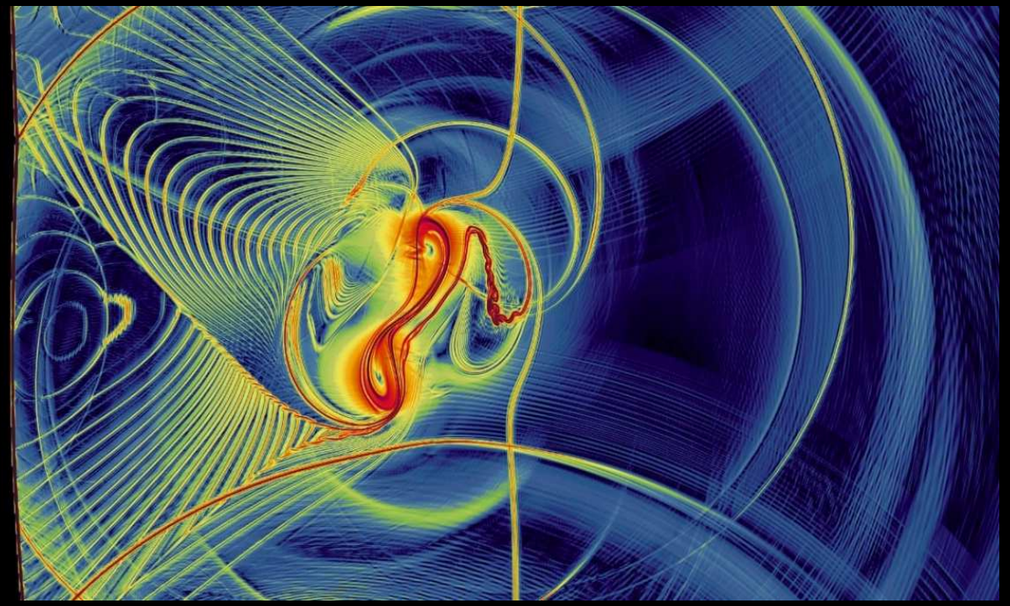
- Three-Phase contact line
- Extended DG for two- and three-phase
- Results
- Other Applications

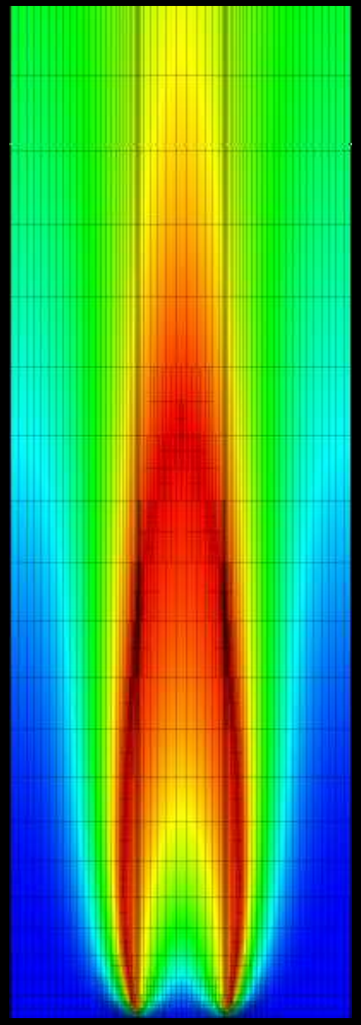
- Future Direction: 3D, HPC

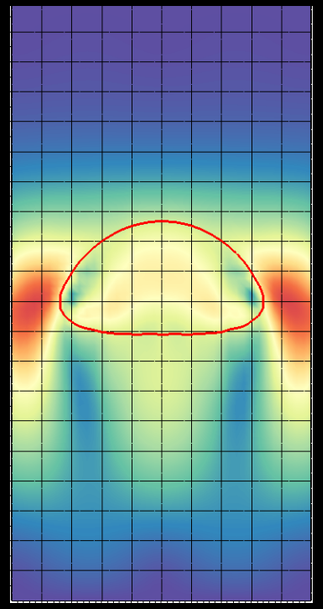
# BoSSS is open source

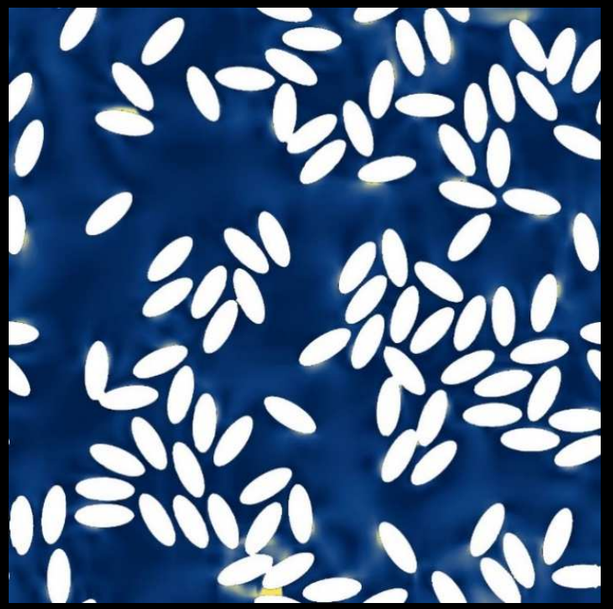
get your copy @ github.com/FDYdarmstadt/BoSSS

TECHNISCHE UNIVERSITÄT DARMSTADT



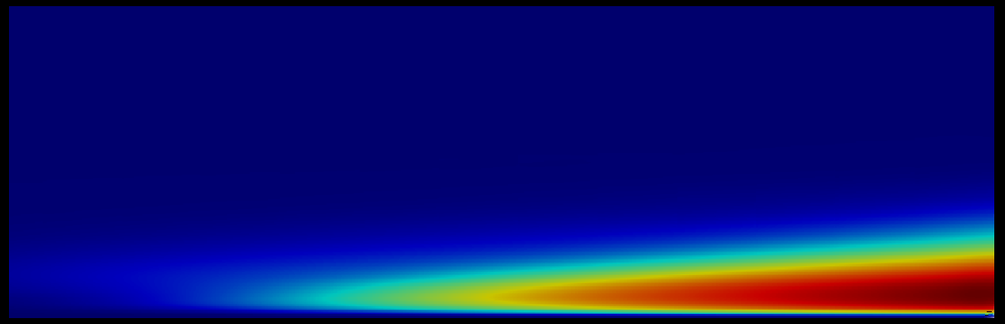


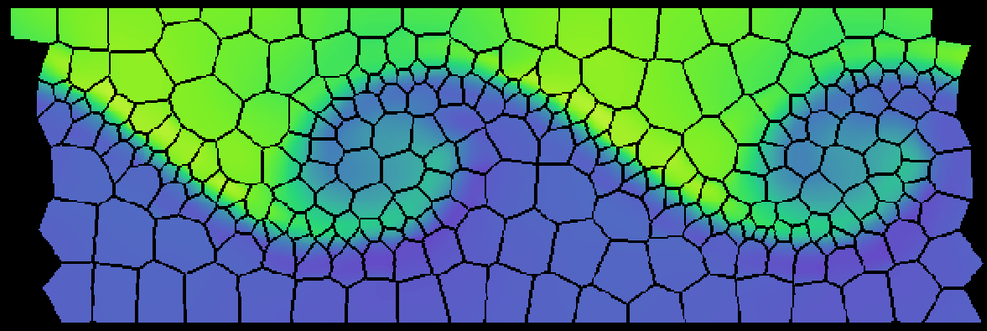




$k$-$\omega$ ▽ compressible △ combustion ▷

△ IBM ▽ Voronoi △ multi-body





TECHNISCHE UNIVERSITÄT DARMSTADT

# THANK YOU FOR YOUR ATTENTION!


Dr. Florian Kummer

**Fachgebiet für Strömungsdynamik**
Technische Universität Darmstadt, L1|01 324
Otto-Berndt-Straße 2
64287 Darmstadt, Germany

FON +49 6151 16-26194
FAX +49 6151 16-26203
Mail: kummer@fdy.tu-darmstadt.de
Homepage: www.fdy.tu-darmstadt.de


MASCHINENBAU
We engineer future FDY