Numerical Simulation of Powder Flow

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- Models for granular flow
- Numerical aspects
- Discussion and outlook

Motivation of our Resarch

‘Preserve the high efficiency of special PDE solvers
for flow problems’

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'Preserve the high efficiency of special PDE solvers for flow problems'

→ **High (guaranteed) accuracy for user-specific quantities !**

→ **With minimal #d.o.f.s !**

→ **Via robust solvers with 'optimal' numerical complexity !**

→ **Exploiting the huge sequential/parallel GFLOP/s rates !**

$$\Downarrow$$

Realization for complex CFD ?

CFD Software FEATFLOW

- Continuum mechanical description, for example

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \mathbf{S} + \rho g \quad , \quad \nabla \cdot \mathbf{u} = 0$$

$$\mathbf{S} = \mu \, \frac{p}{\epsilon + |\mathbf{D}(\mathbf{u})|} \, \mathbf{D}(\mathbf{u}) \quad , \quad \mu = \sqrt{2} \sin \phi$$

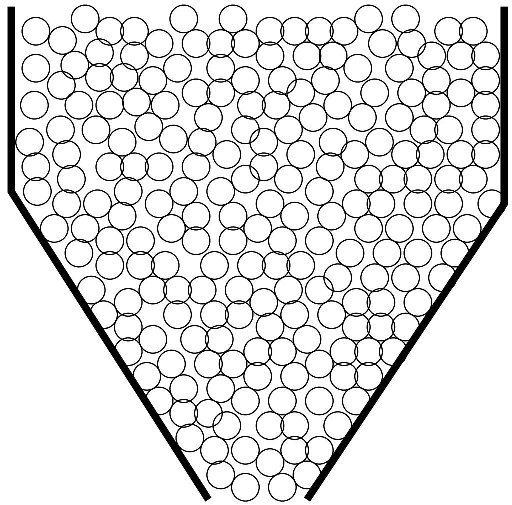
- Finite Elemente methods, iterative solvers

‘Nonlinear models for granular flow based on generalized Navier-Stokes equations’

$$\mathbf{S} = \nu(\mu, p, D(\mathbf{u})) \, \mathbf{D}(\mathbf{u})$$

Application to Granular Flow

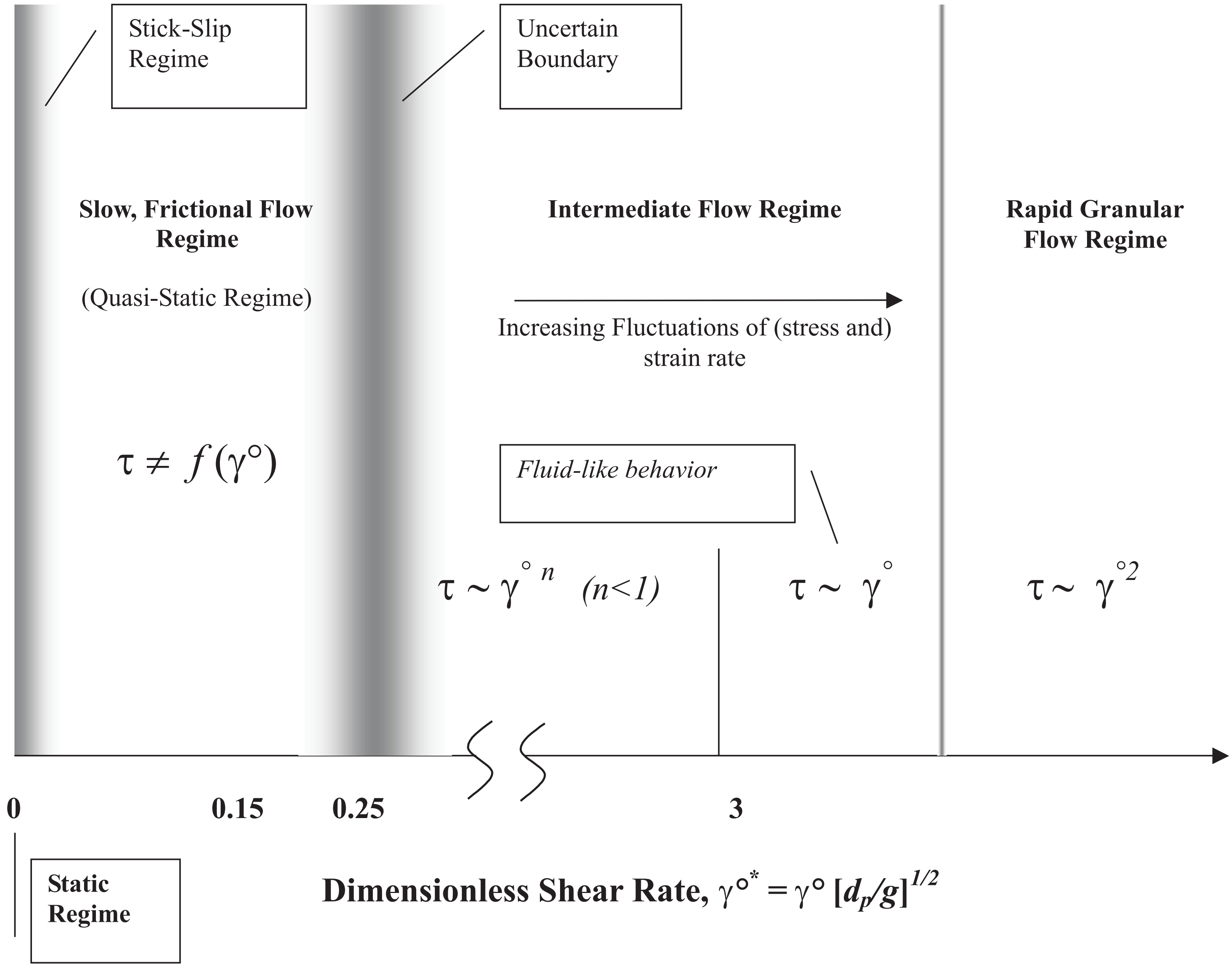
Pharmaceutical Industry, Food Processing, Soil Mechanics



The behaviour of **granular flow** *is different from that of fluids since it does not exhibit* **viscosity** *and the dominant interaction between particles is* **friction**. *[Nevertheless, numerical methods are similar.]*

We do not examine flow of large grains but **smaller-sized bulk powders** *where a* **continuum approach** *may be more advantageous.*
[$\longrightarrow$ generalized Navier-Stokes equations]

Regimes of Powder Flow (cf. Tardos)



Static Regime

Assumption: The flow is slow enough so that any movement between 2 static states can be neglected.

Advantages:

- static ‘equilibrium’ equation can be applied
- theory predicts the onset of flow

Disdvantages:

- no flow field can be predicted
- no flow rates result from theory

‘Method of Slices’ (Jenkins 1895)
It is (still) used for the design of silos !

Slow, Frictional Regime

General equations of flow result from:

- adding inertial effects to the static equations
- considerations of continuity
- using a yield condition
- invoking a "flow rule"

(Most) Important from industrial point of view !

First model: Schaeffer (1987)

Intermediate + Rapid-Granular Regimes

Intermediate: Both inter-particle friction and collisional energies are important.

$\rightarrow$ **More research needed !**

Rapid-Granular: Short particle-particle contacts are important while frictional forces are neglected; particles behave as molecules in a dense gas.

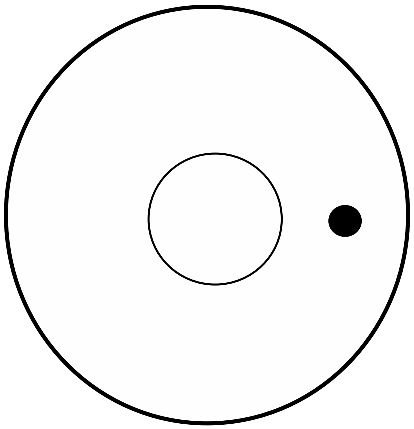
Equations of flow result from a 'Kinetic Theory' type model:

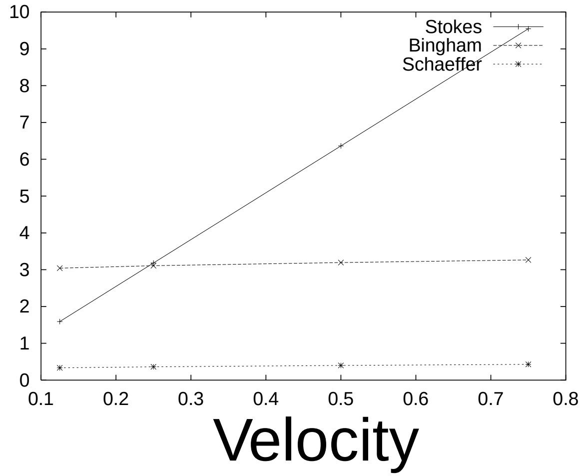
- conservation of mass
- conservation of momentum
- conservation of energy

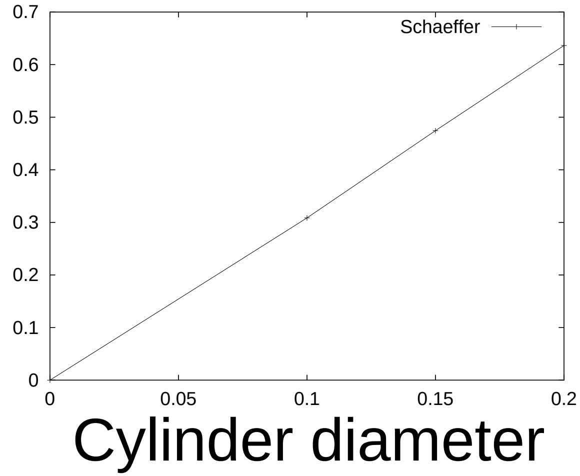
Characteristics of Slow Granular Flow

- Open a silo hopper and.....???

- The **drag force** for Schaeffer and Bingham flow acting on a cylinder is **independent** of the grain **velocity**, contrary to Stokes flow







When mechanical ploughs replaced draught animals, it was observed that ploughing at greater speeds does not require greater forces! (Schaeffer)

General Powder Flow Model

- **Conservation of mass** ($\mathbf{u}$ is the velocity vector)

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\mathbf{u}) = 0$$

- **For an incompressible material** the bulk density, ρ, is a constant:

$$\nabla \cdot \mathbf{u} = 0$$

- **Equation of motion**

$$\rho\frac{Du}{Dt} = -\nabla \cdot \mathbf{T} + \rho g$$

with $\mathbf{T} = \mathbf{S} + p\mathbf{I}$ ("stress field" T, deviatoric part S, pressure p)

Constitutive Equations

The **constitutive equation** is devoted to correlate between the **deviatoric tensor** S and the **velocity** $\mathbf{u}$, through the **rate of deformation** $\mathbf{D} = \frac{1}{2}(\nabla \mathbf{u} + \nabla^T \mathbf{u})$, and to assure the closure of the equations.

- **Newtonian law**

$$\mathbf{S} = 2\nu_{\mathrm{o}}\mathbf{D}$$

- **Power law**

$$\mathbf{S} = 2\nu(\|\mathbf{D}\|^2)\mathbf{D}, \quad \nu(z) = z^{\frac{r}{2}-1}, \quad r > 1$$

- **Schaeffer's law (1987):** For a powder a constitutive equation was first introduced by Schaeffer (1987), which has to obey a
  - von Mises yield condition; $\|\mathbf{S}\| = \sqrt{2}p\sin\phi$, and
  - Levy's flow rule; $\mathbf{S} = \lambda\mathbf{D}$.

  We use this correlation to obtain the constitutive equation

$$\mathbf{S} = \sqrt{2}p\sin\phi\frac{\mathbf{D}}{\|\mathbf{D}\|}$$

Generalized Navier-Stokes Equations

The generalized incompressible Navier-Stokes problem reads:

$$\rho \frac{Du}{Dt} = -\nabla p + \nabla \cdot (\nu(p, D_{\mathrm{II}})\mathbf{D}) + \rho g, \quad \nabla \cdot \mathbf{u} = 0$$

If we define the 'pseudo viscosity' $\nu(\cdot,\cdot)$ as function of $D_{\mathrm{II}}(u) = \frac{1}{2}\mathbf{D} : \mathbf{D}$ and p, we obtain a full range of different 'nonlinear flow models':

- **Power law** defined for

$$\nu(z, p) = \nu_0 z^{\frac{r}{2}-1}$$

- **Bingham law** defined for

$$\nu(z, p) = \nu_0 z^{-\frac{1}{2}}$$

- **Schaeffer's law** (including the pressure) defined for

$$\nu(z, p) = \sqrt{2} \sin\phi \, p z^{-\frac{1}{2}}$$

- ...other laws with pressure-dependent viscosity...

Mathematical Challenges I

- **Mathematical Analysis:**
  For pressure-dependent viscosity: Hron/Malek/Necas/Rajagopal, Schaeffer

- **Discretization method:**
  LBB-stable FEM discretization?
  Uniqueness of the pressure? Inflow profiles?
  Operator-Splitting (a la Chorin, Van Kan)?

- **Nonlinear solver:**
  Newton techniques for this highly nonlinear problem?
  Decoupling of pressure and velocity?

- **Linear multigrid solver:**
  New types of saddle-point problems?

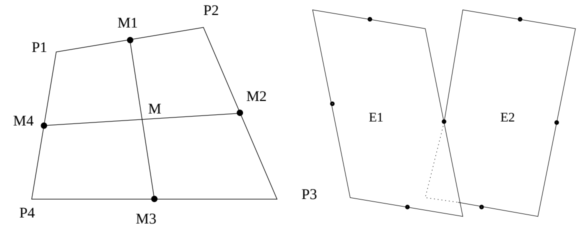
Mathematical Challenges II

1. **Discretization method:** The approximation of incompressible velocity fields is subject to the so-called
   - **LBB-condition**
   $$\min_{q_h \in Q_h} \max_{\mathbf{v}_h \in V_h} \frac{(q_h, \nabla \cdot \mathbf{v}_h)}{\|q_h\|_0 \|\nabla \mathbf{v}_h\|_0} \geq \beta > 0, \tag{1}$$
   - **Discrete Korn's inequality**
   $$\sum_{\tau \in \tau_h} \|v\|_{H^1(\tau)} \leq c(\|v\|_{L^2}^2 + \|D(v)\|_{L^2}^2)^{\frac{1}{2}} \tag{2}$$
2. **Convection-dominated transport** specially at high Reynolds number ($Re = \frac{1}{\nu}$)
3. **Boundary condition**

Spatial Discretization

Quadrilateral Rannacher-Turek Stokes Element

$$\tilde{Q}_1 := \{q \circ \psi_T^{-1} : q \in \text{span} < 1, x, y, x^2 - y^2 >\}$$



The degree of freedom are determined by the nodal functionals

$$\{F_\Gamma^{(a,b)}(\cdot), \Gamma \subset \partial \mathcal{T}_h\}, \text{ with}$$

$$F_\Gamma^a := |\Gamma|^{-1} \int_\Gamma v d\gamma \quad \text{or} \quad F_\Gamma^b := v(m_\Gamma) \quad (m_\Gamma \text{ midpoint of edge } \Gamma) \tag{3}$$

- Advantage
  - Stable and efficient for incompressible flow.
  - Compact data structures.
- Disadvantage
  - Not satisfying **classical** discrete Korn's inequality
  - Numerical oscillations for convection dominated problem

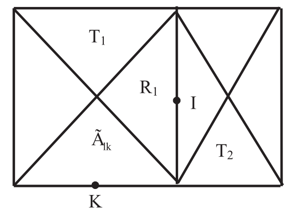
Classical Stabilization Methods

- FEM streamline diffusion

$$\langle \tilde{\mathbf{N}}(\mathbf{u})\mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{N}(\mathbf{u})\mathbf{v}, \mathbf{w} \rangle + \langle \mathbf{N}_{sd}(\mathbf{u})\mathbf{v}, \mathbf{w} \rangle \quad , \qquad \text{where} \tag{4}$$

$$\langle \mathbf{N}_{sd}(\mathbf{u})\mathbf{v}, \mathbf{w} \rangle = \sum_{T \in T_h} \delta_T \int_T (\mathbf{u} \cdot \nabla \mathbf{v})(\mathbf{u} \cdot \nabla \mathbf{w})\, dx. \tag{5}$$

- FEM upwinding



$$\langle \tilde{\mathbf{N}}(\mathbf{u})\mathbf{v}, \mathbf{w} \rangle = \sum_l \sum_{k \in \Lambda_l} \oint_{\Gamma_{lk}} \mathbf{u} \cdot \mathbf{n}_{lk} d\gamma \; [1 - \lambda_{lk}(\mathbf{u})(\mathbf{v}(m_k) - \mathbf{v}(m_l))]\mathbf{w}(m_l) \tag{6}$$

Based on the local Reynolds number $Re_\tau = \frac{\|\mathbf{u}\|_\tau \cdot h_h}{\nu}$,
we can either define

$$\delta_\tau = \delta^* \cdot \frac{h_\tau}{\|\mathbf{u}\|_\Omega} \cdot \frac{2Re_\tau}{1 + Re_\tau}, \qquad \lambda_{lk}(u_h) = \begin{cases} \dfrac{\frac{1}{2} + \delta^* Re_\tau}{1 + \delta^* Re_\tau} & \textit{\textbf{if}}\ Re_\tau \geq 0 \\[2ex] \dfrac{1}{2(1 - \delta^* Re_\tau)} & \textit{\textbf{otherwise}} \end{cases} \tag{7}$$

New Edge-oriented FEM Stabilization

- **Based only on the "smoothness" of the discrete solution** we have developed the following jump term

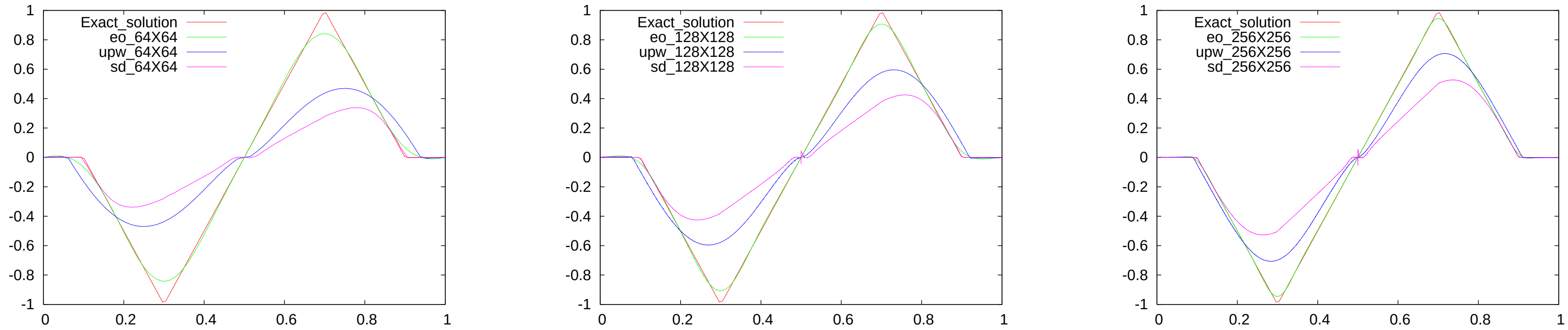
$$\sum_{\text{edge } E} \max(\gamma\nu h_E, \gamma^* h_E^2) \int_E [\nabla \mathbf{u}][\nabla \mathbf{v}] d\sigma \quad \text{with} \gamma, \gamma^* \in [0.0001, 0.1] \tag{8}$$

- Only one generic stabilization takes care of all instabilities
  1. due to Korn's inequality
  2. due to convection dominated flow for medium and high Reynolds number, even for pure transport
  3. due to problems with variable viscosity

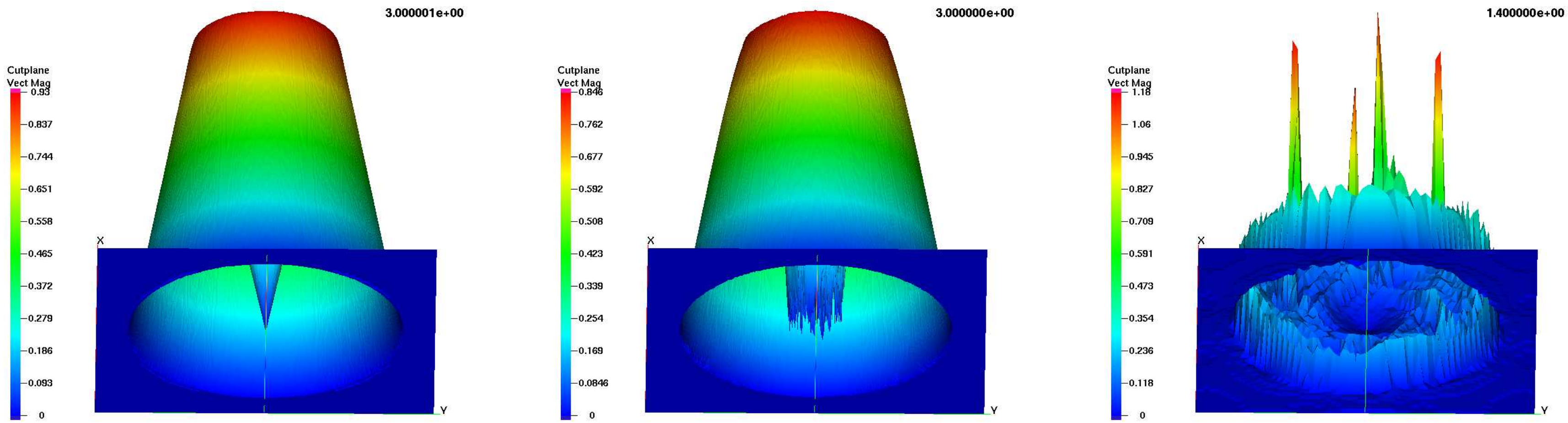
- **Independent of the local Reynolds number**

Standing vortex $Re = \infty$

- Cutline of the x-velocity component for the ‘Standing Vortex’ problem



- 3D presentation of the norm of the velocity (VECT MAG) for the ‘Standing Vortex’ problem: edge-oriented (left) vs. streamline-diffusion (middle) and central (right)



- **Upwind: significant smearing effects**
- **EO: preserves “perfectly” the solution with high accuracy**

Nonlinear Solver: Newton Iteration

Let $\mathbf{u}^l$ being the initial state, the (continuous) Newton method consists of finding $\mathbf{u}$ such that

$$\int_\Omega 2\nu(D_{\mathbf{I}}(\mathbf{u}^l), p^l)\mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v})dx$$

$$+ \int_\Omega 2\partial_1\nu(D_{\mathbf{I}}(\mathbf{u}^l), p^l)[\mathbf{D}(\mathbf{u}^l) : \mathbf{D}(\mathbf{u})][\mathbf{D}(\mathbf{u}^l) : \mathbf{D}(\mathbf{v})]dx$$

$$+ \boxed{\int_\Omega 2\partial_2\nu(D_{\mathbf{I}}(\mathbf{u}^l), p^l)[\mathbf{D}(\mathbf{u}^l) : \mathbf{D}(\mathbf{v})]p dx}$$

$$= \int_\Omega \boldsymbol{f}\mathbf{v} - \int_\Omega 2\nu(D_{\mathbf{I}}(\mathbf{u}^l), p^l)\mathbf{D}(\mathbf{u}^l) : \mathbf{D}(\mathbf{v})dx, \quad \forall \mathbf{v}, \quad (9)$$

where $\partial_i\nu(\cdot,\cdot); i = 1, 2$ is the partial derivative of ν related to the first and second variable, respectively.

New Linear Algebraic Problem

Every Newton step consists of finding $(\mathbf{u}, p)$ as solution of the linear system

$$\begin{cases} A(\mathbf{u}^l, p^l)\mathbf{u} + \delta_u A^*(\mathbf{u}^l, p^l)\mathbf{u} + Bp + \delta_p B^*(\mathbf{u}^l, p^l)p & = R_u(\mathbf{u}^l, p^l), \\ B^T\mathbf{u} & = R_p(\mathbf{u}^l, p^l), \end{cases} \tag{10}$$

where $R_u(\cdot, \cdot)$ and $R_p(\cdot, \cdot)$ denote the corresponding nonlinear residual terms for the momentum and continuity equations, and the matrix $A^*(\mathbf{u}^l, p^l)$ and $B^*(\mathbf{u}^l, p^l)$ are defined as follows, respectively

$$\langle A^*(\mathbf{u}^l, p^l)\mathbf{u}, \mathbf{v}\rangle = \int_\Omega 2\partial_1 \nu(D_{\|}(\mathbf{u}^l), p^l)[D(\mathbf{u}^l) : D(\mathbf{u})][D(\mathbf{u}^l) : D(\mathbf{v})]dx. \tag{11}$$

$$\boxed{\langle B^*(\mathbf{u}^l, p^l)p, \mathbf{v}\rangle = \int_\Omega 2\partial_2 \nu(D_{\|}(\mathbf{u}^l), p^l)[D(\mathbf{u}^l) : D(\mathbf{v})]p dx.} \tag{12}$$

Schaeffer Model (I)

The nonlinear 'pseudo viscosity' has the form $\nu(p,z) = Q(p)z^{\frac{r}{2}-1}$

- New type of (nonsymmetric) saddle-point problems;

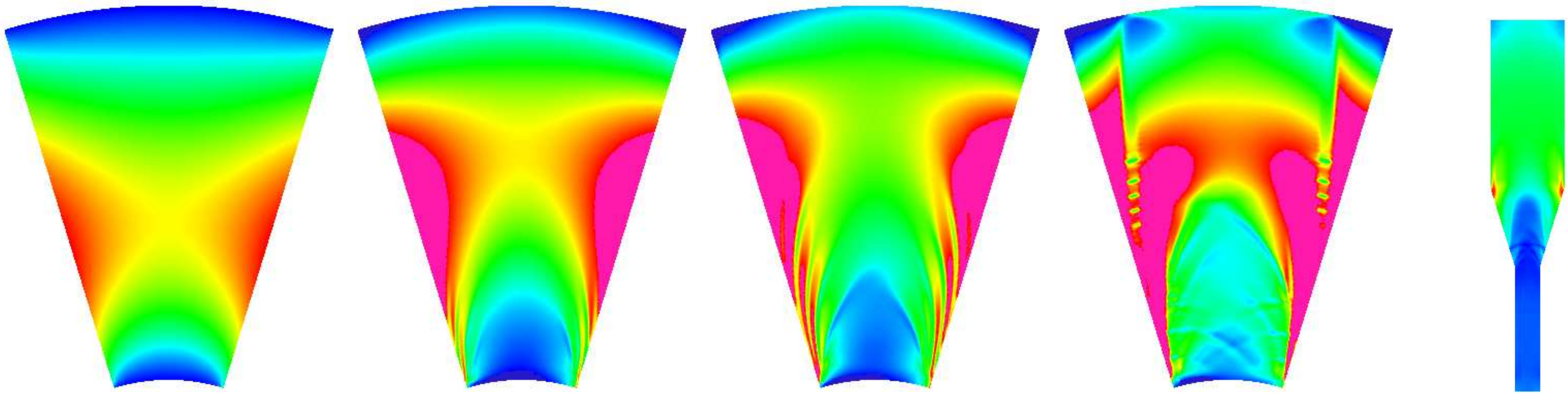
$$M_{\delta_p}(\tilde{\mathbf{u}},\tilde{p}) = \begin{pmatrix} A_u & B + \delta_p B^* \\ B^T & 0 \end{pmatrix}$$

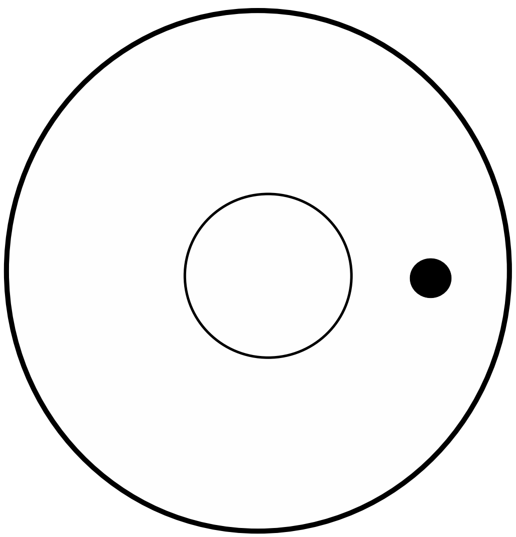
- The (linear) solution depends on the choice of imposing the uniqueness, since $\dim($null$(M_{\delta_p})) = 1$

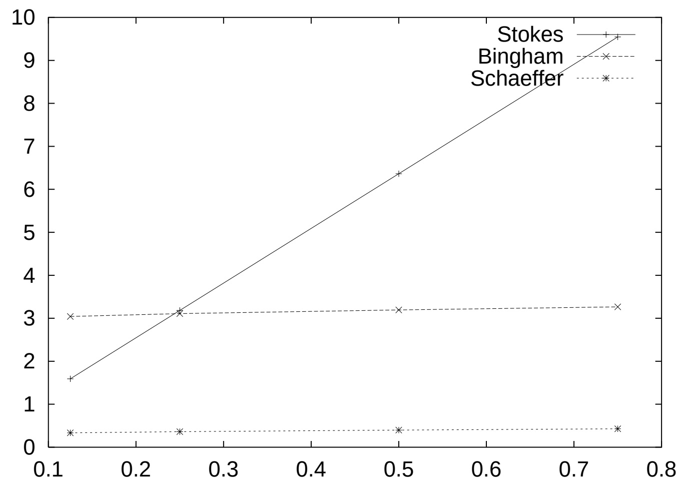
$\nu = \frac{exp(\beta p)}{\epsilon + \|\mathbf{D}(\mathbf{u})\|}$		
β	Newton	Fixed Point
5×10^{-2}	$10/3$	$200/1$
1×10^{-1}	$11/3$	$250/1$
2×10^{-1}	$10/3$	$238/2$

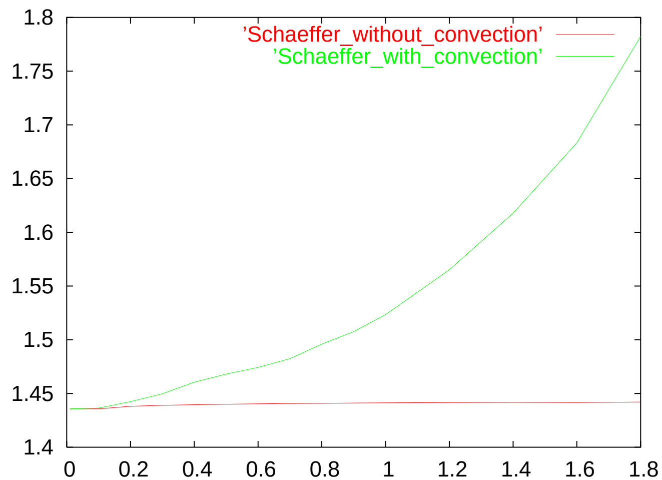
$\nu = \frac{\beta p}{\epsilon + \|\mathbf{D}(\mathbf{u})\|}$	
Newton	Fixed Point
$12/13$	$405/2$
$12/10$	$522/2$
$12/10$	$581/2$

Konfigurationen









Schaeffer Model (II)

- **Schaeffer's law:** The nonstationary equations are **linearly ill-posed** according to Schaeffer.
- **Flow rate:** The quantitative prediction of the flow rate through silo hoppers is wrong by more than 100%
- **Add compressibility:** This approach is an effort to regularize the instability.

Compressible Powder Models (cf. Tardos)

- **General equation of motion for a powder**

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \left[\frac{q(p,\rho)}{\|\mathbf{D} - \frac{1}{n}\nabla \cdot \mathbf{u} I\|} \left(\mathbf{D} - \frac{1}{n}\nabla \cdot \mathbf{u} I\right) \right] + \rho g, \text{ with}$$

- **Continuity equation**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \text{ and}$$

- **Normality condition**

$$\nabla \cdot \mathbf{u} = \frac{\partial q(p,\rho)}{\partial p} \|\mathbf{D} - \frac{1}{n}\nabla \cdot \mathbf{u} I\|$$

- **Yield condition $q(p,\rho)$ is given by:**

Powder properties	Non-cohesive	Cohesive
Incompressible	$p \sin\phi$	$p \sin\phi + c\cos\phi$
Compressible	$p \sin\phi \left[2 - \frac{p}{\rho^{\frac{1}{\beta}}} \right]$	$p \sin\phi \rho^{\frac{1}{\beta}} - C \frac{(p - \rho^{\frac{1}{\beta}})^2}{\rho^{\frac{1}{\beta}}}$

Summary:

- More mathematical research is needed to understand and to analyse the models for granular and powder flows.
- Numerical analysis of discretization and solution techniques?
- The physically correct choice of pressure (mean)values is not clear.
- How to prescribe velocity profiles? [Or: Fluxes?]

Outlook I: Hypoplastic Model by Kolymbas

$$\text{Re}\,[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}] = -\nabla p + \nabla\cdot\mathbf{S} + \mathbf{f} \quad , \quad \nabla\cdot\mathbf{u} = 0$$

$$\mathbf{S} = \frac{Q(p)}{|\mathbf{D}(\mathbf{u})|}\mathbf{D}(\mathbf{u}) \text{ (Schaeffer/Power Law/etc.) } + \mathbf{T} \text{ (Kolymbas)}$$

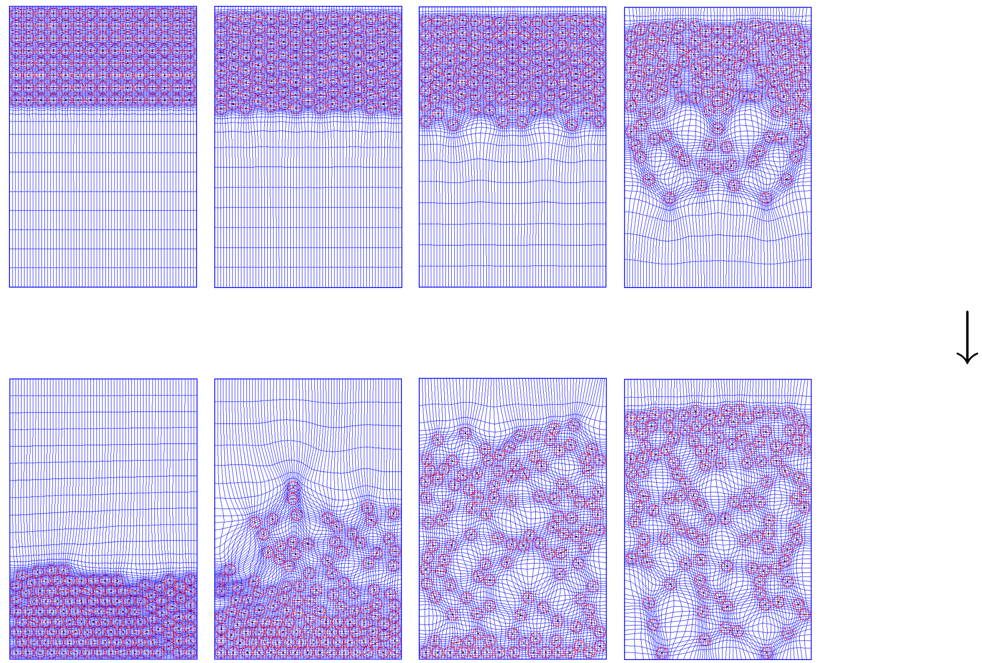
$$\begin{aligned} \frac{\partial \mathbf{T}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{T} \quad = \quad & -[\mathbf{TW} - \mathbf{WT}] + C_1\frac{1}{2}(\mathbf{TD} - \mathbf{DT}) \\ & + C_2 tr(\mathbf{TD})\cdot\mathbf{I} + C_3\sqrt{tr\mathbf{D}^2}\mathbf{T} + C_4\frac{\sqrt{tr\mathbf{D}^2}}{tr\mathbf{T}}\mathbf{T}^2 \\ & + \nu(\mathbf{D})[\frac{\partial \mathbf{D}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{D} + \mathbf{DW} - \mathbf{WD}] \end{aligned}$$

1. FEM discretization and solver ?
2. Free boundary ? Fluid-Structure interaction ?
3. Numerical ‘falsification’ of material/flow models !?

Outlook II: Particulate Flow

Development of simulation tools for the understanding of:

1. Interaction of solid particles with flow ($\longrightarrow$ many complex objects ?)
2. Behaviour of nonlinear fluid models



- ‘Fictitious Boundary Method’ on adapted meshes + Operator-Splitting !
- ‘Many’ particles ? Nonlinear fluids ? Wide range of applications !