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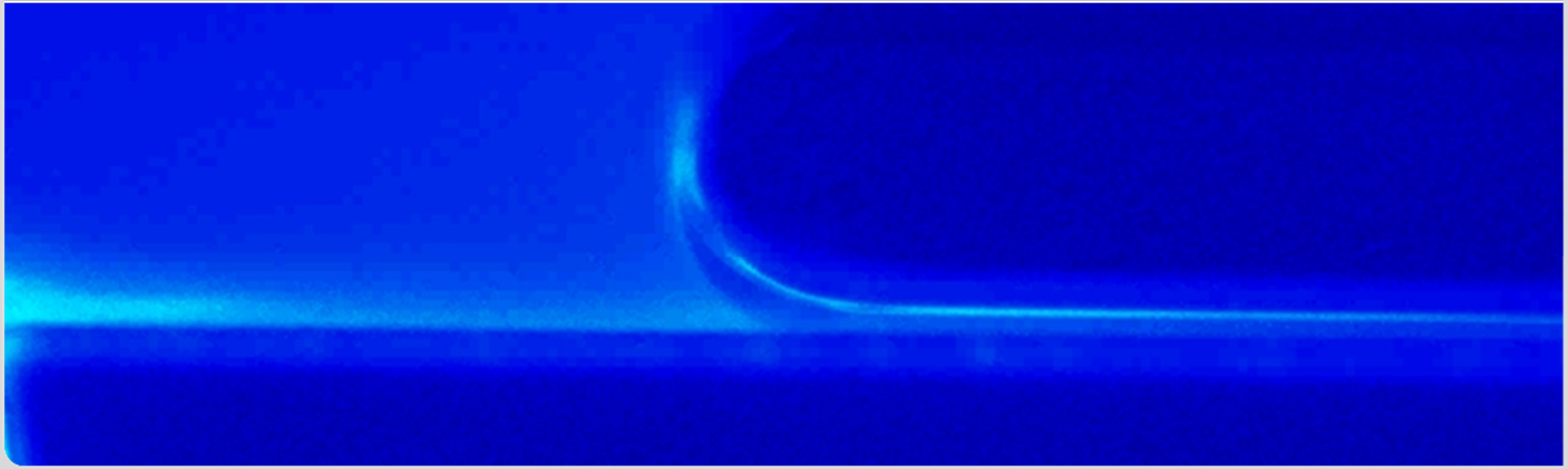
Transport processes at fluidic interfaces
DFG SPP 1506

Development of a simulation method for mass transfer in two-fluid flows

Carlos Falconi, Martin Wörner

DFG-SPP 1506: Transport processes at fluidic interfaces

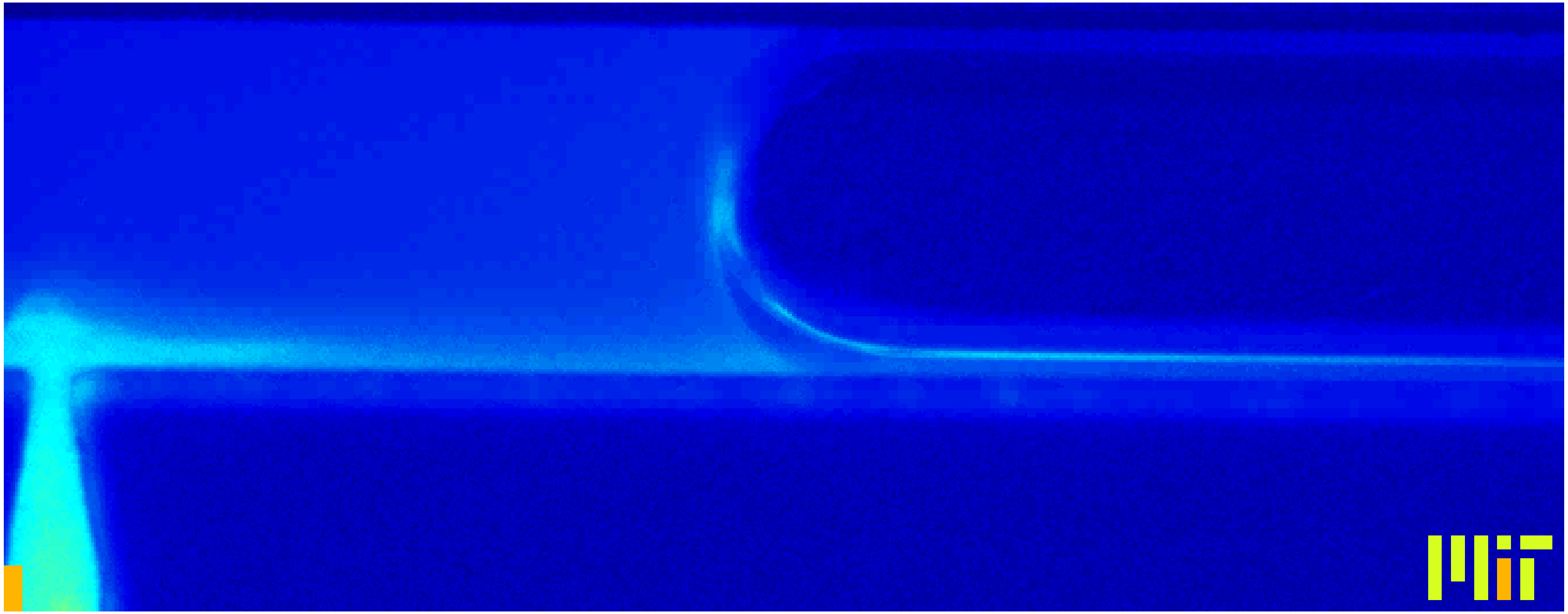
Institute for Nuclear and Energy Technologies (IKET), KIT-Campus North



Outline

- Motivation
  - Taylor flow and physical phenomena
  - DNS: Difficulties and limitations
- Simulation method
  - Hydrodynamic equation
  - Species conservation equation
  - Hierarchical grid method
  - Development of interpolation algorithms
- Outlook

Taylor flow

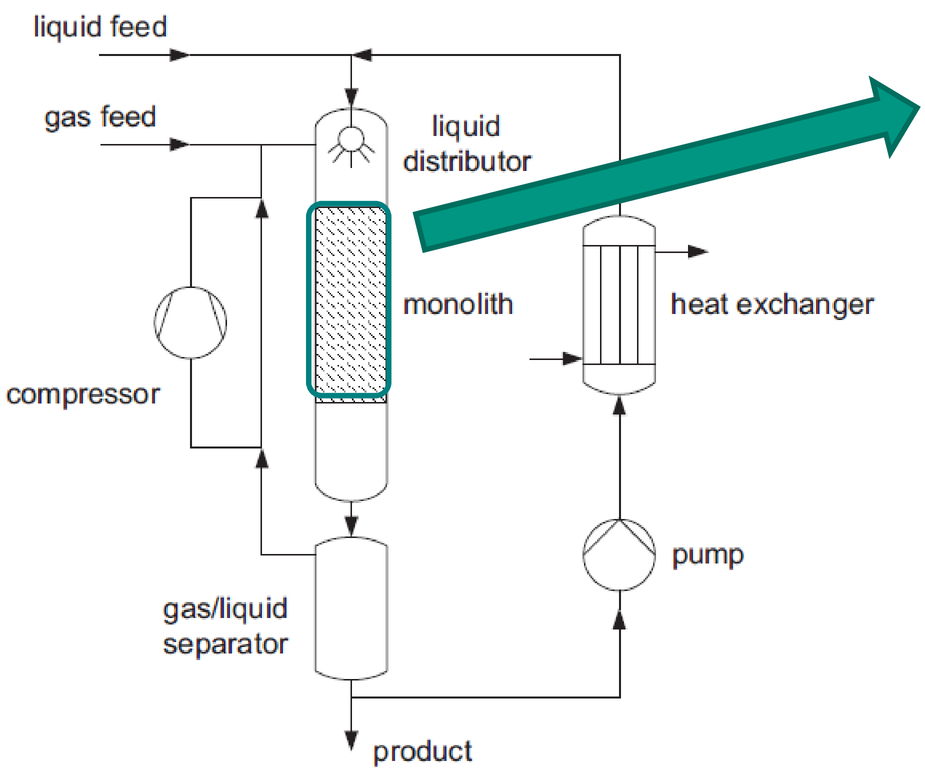


Channel cross section are: 400 µm × 280 µm

*Movie of Günther et al. Langmuir **21** (2005) 1547-1555*

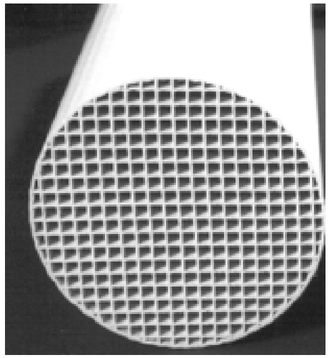
Industrial application

- Catalyst monolithic reactor with Taylor flow
  - Production of synthetic fuels by Fischer-Tropsch synthesis (2ph. flow)

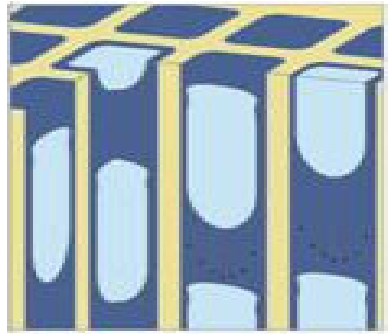


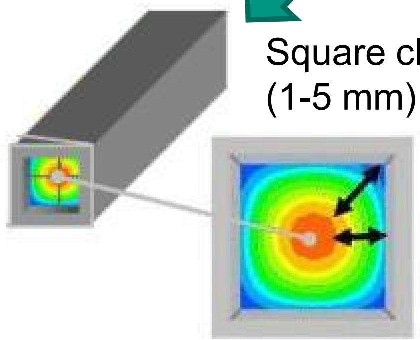
Monolith-Loop-Reaktor
Heiszwolf et al. (2001)

Monolith



2-phase flow



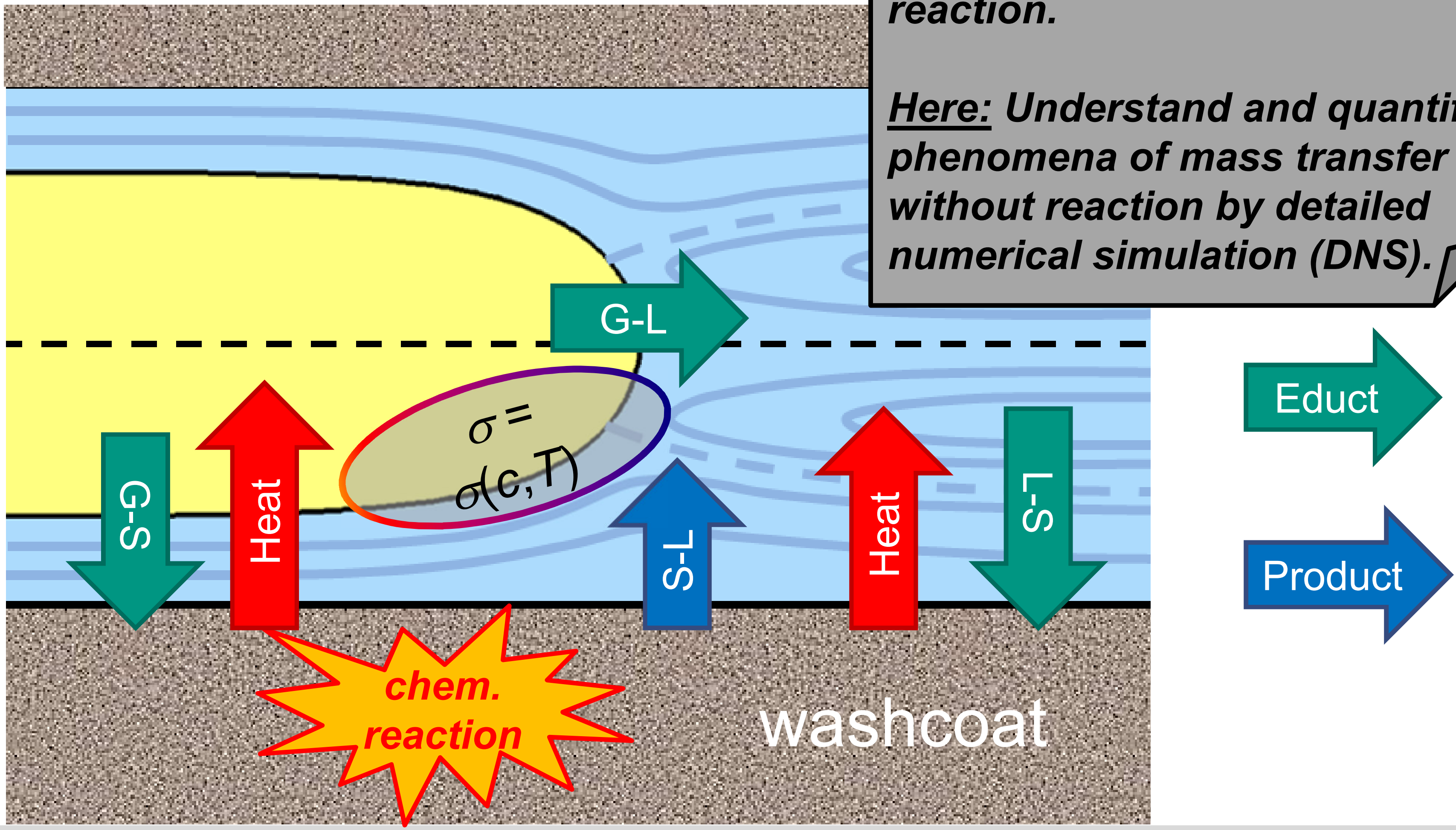


Square channels
(1-5 mm)

Physical phenomena

Complex non-linear coupling between flow, transport and reaction.

<u>Here:</u> Understand and quantify phenomena of mass transfer without reaction by detailed numerical simulation (DNS).



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Karlsruhe Institute of Technology (KIT) - Campus North

Difficulties and limitations

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Boundary layer thickness at the moving interface

State of the arts:

2D: Sc ≈ 50 (Khinast), uniform concentration in gas

3D: Sc ≈1 (Onea, Wörner), Conjugated mass transfer

3D: Sc ≈1000 (Bothe),

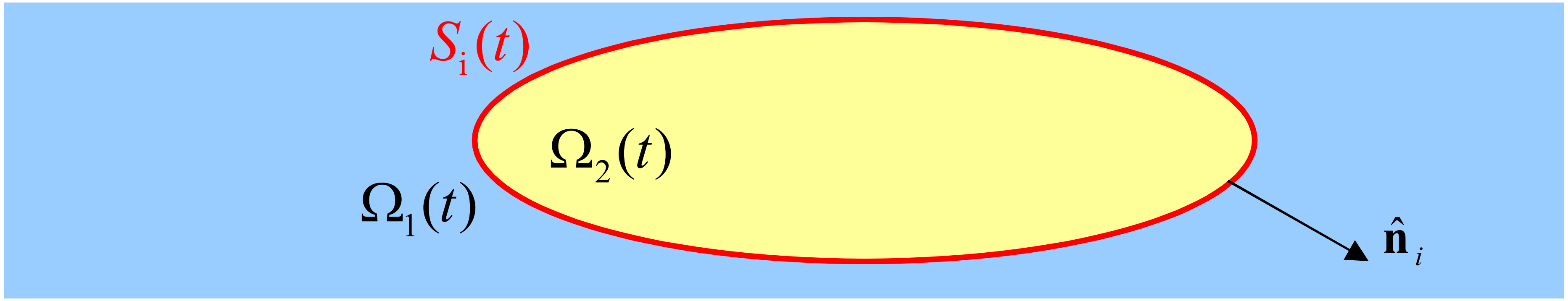
Subgrid scales model, uniform concentration in gas

GOAL: 3D: Sc = 50, Conjugated mass transfer

Outline

- Motivation
  - Taylor flow and physical phenomena
  - DNS: Difficulties and limitations
- Simulation method
  - Model assumptions
  - Hydrodynamic equation
  - Species conservation equation
  - Hierarchical grid method
  - Development of interpolation algorithm
- Outlook

Model assumptions



Single-field momentum eq.

$\Omega = \Omega_1 + \Omega_2$

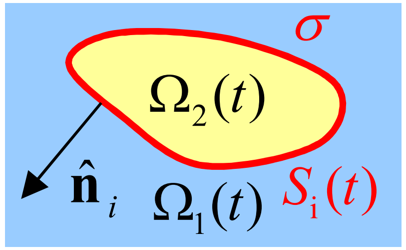
$$\frac{\partial f}{\partial t} + \nabla \cdot f\,\mathbf{v}_\mathrm{m} = 0 \qquad \nabla \cdot \mathbf{v}_\mathrm{m} = 0$$

$f \equiv 1,\ \mathbf{x} \in \Omega_1(t)$

$f \equiv 0,\ \mathbf{x} \in \Omega_2(t)$

$1 < f < 0,\ \mathbf{x} \in S_i(t)$

0.493	0.493	0.177	0.0
1.0	1.0	0.925	0.177
1.0	1.0	1.0	0.493
1.0	1.0	1.0	0.493



$$\frac{\partial \rho_\mathrm{m} \mathbf{v}_\mathrm{m}}{\partial t} + \nabla \cdot \left(\rho_\mathrm{m} \mathbf{v}_\mathrm{m} \mathbf{v}_\mathrm{m}\right) = -\nabla P + \frac{\nabla \cdot \left[\mathbb{T}_m\right]}{Re_\mathrm{ref}} + \left[f + (1-f)\frac{\rho_2}{\rho_1}\right] Fr_\mathrm{ref}\,\hat{\mathbf{e}}_\mathrm{g} + \frac{Eu_\mathrm{ref}}{L_\mathrm{axial}}\hat{\mathbf{e}}_\mathrm{axial} + \frac{a_\mathrm{i}\kappa\hat{\mathbf{n}}_\mathrm{i}}{We_\mathrm{ref}}$$

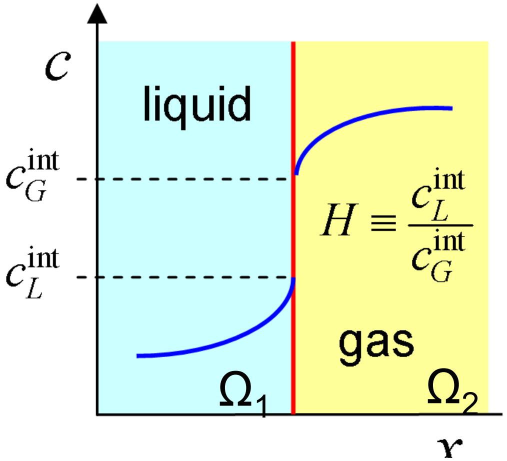
$$\mathbb{T}_m = \nabla \cdot \left[\mu_\mathrm{m}\left(\nabla \mathbf{v}_\mathrm{m} + \left(\nabla \mathbf{v}_\mathrm{m}\right)^\mathrm{T}\right)\right],\ \mathbf{v}_\mathrm{m} \equiv \frac{f\rho_1 \overline{\mathbf{v}_1}^{V_1} + (1-f)\rho_2 \overline{\mathbf{v}_2}^{V_2}}{\alpha_1\rho_1 + \alpha_2\rho_2},\quad \rho_\mathrm{m} \equiv f\rho_1 + (1-f)\rho_2,\quad \mu_\mathrm{m} \equiv f\mu_1 + (1-f)\mu_2$$

$$a_i = (A_i / V) \qquad \kappa = -\nabla \cdot \hat{\mathbf{n}}_i$$

- **Assumptions:**
  - $p_m = p_1 = p_2 = P$
  - Interface curvatures and all scales are well resolved
  - $V_r = 0$

Solution with the volume of fluid method (VOF) with geometrical interface reconstruction (EPIRA)

Single-field mass transfer eq.



$$c_{1i} = H c_{2i} \;, \mathbf{x} \in S_i \left(t\right)$$

$\Omega = \Omega_1 + \Omega_2$

Normal single field fomulation

$$\frac{\partial c_{\mathrm{m}}}{\partial t} + \nabla \cdot \left(c_{\mathrm{m}} \mathbf{v}_{\mathrm{m}}\right) = -\frac{1}{Re_{\mathrm{ref}} Sc_{\mathrm{ref}}} \left[\nabla \cdot \mathbf{j}_{\mathrm{m}}\right]$$

$$\mathbf{j}_{\mathrm{m}} \equiv -D_{\mathrm{m}} \nabla c_{\mathrm{m}}$$

$$D_{\mathrm{m}} \equiv f D_{\mathrm{L}} + (1-f) D_{\mathrm{G}}, \; c_{\mathrm{m}} \equiv f c_{\mathrm{L}} + (1-f) \; c_{\mathrm{G}}$$

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Coupling of the system

1) Volume fraction eq.

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

2) N.S.eq.

conservation of mass

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

conservation of momentum

$$\frac{\partial \rho_\mathrm{m} \mathbf{v}_\mathrm{m}}{\partial t} + \nabla \cdot \left(\rho_\mathrm{m} \mathbf{v}_\mathrm{m} \mathbf{v}_\mathrm{m}\right) = -\nabla P + \frac{\nabla \cdot \left[\nabla \cdot \left[\mu_\mathrm{m}\left(\nabla \mathbf{v}_\mathrm{m} + \left(\nabla \mathbf{v}_\mathrm{m}\right)^\mathrm{T}\right)\right]\right]}{Re_\mathrm{ref}}$$

$$+\left[f + \left(1-f\right)\frac{\rho_2}{\rho_1}\right] Fr_\mathrm{ref} \hat{\mathbf{e}}_\mathrm{g} + \frac{Eu_\mathrm{ref}}{L_\mathrm{axial}} \hat{\mathbf{e}}_\mathrm{axial} + \frac{a_\mathrm{i} \kappa \hat{\mathbf{n}}_\mathrm{i}}{We_\mathrm{ref}}$$

3) Species transport eq.

$$\frac{\partial c_\mathrm{m}}{\partial \theta} + \nabla \cdot \left(c_\mathrm{m} \mathbf{v}_\mathrm{m}\right) = -\frac{1}{Re_\mathrm{ref} Sc_\mathrm{ref}}\left[-\nabla\left(D_\mathrm{m} \nabla c_\mathrm{m}\right) + (1-H) a_\mathrm{i} j_\mathrm{i}\right]$$

$$\mathbf{v}_\mathrm{m} \equiv \frac{f \rho_1 \overline{\mathbf{v}_1}^{V_1} + \left(1-f\right)\rho_2 \overline{\mathbf{v}_2}^{V_2}}{\alpha_1 \rho_1 + \alpha_2 \rho_2}, \quad c_\mathrm{m} \equiv f c_\mathrm{L} + (1-f) H c_\mathrm{G}$$

$$\rho_\mathrm{m} \equiv f \rho_1 + \left(1-f\right)\rho_2, \quad \mu_\mathrm{m} \equiv f \mu_1 + \left(1-f\right)\mu_2, \quad D_\mathrm{m} \equiv f D_\mathrm{L} + (1-f) D_\mathrm{G}$$

Flow chart of the simulation

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Hydrodynamic eq.

volume fraction eq.
$v_m^{(n)}, f^{(n)} \rightarrow f^{(n+1)}$
$\rightarrow \rho_m^{(n+1)}, \mu_m^{(n+1)}$

↓

N.S.-eq. without pressure
$\rho_m^{(n+1)}, \mu_m^{(n+1)}, \mu_m^{(n)}, \rho_m v_m^{(n)}$
$\rightarrow \rho_m v_m(*)$

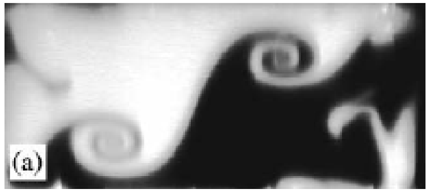
↓

calculation of the pressure (Poisson-eq.)
$v_m(*), p^{(n)} \rightarrow p^{(n+1)}$

↓

correction eq.
$\rho_m v_m(*), p^{(n+1)} \rightarrow v_m^{(n+1)}$

Hydrodynamic. eq. + mass transfer eq. (species)



1 grid

- volume fraction eq.
- N.S.-eq. without pressure
- calculation of the pressure (Poisson-eq.)
- correction eq. $\rightarrow v_m^{(n+1)}$

↓

mass transfer eq.
$c_m^{(n)}, D_m^{(n)}, v_m^{(n+1)} \rightarrow c_m^{(n+1)}$

$$\frac{\delta_c}{\delta_u} = \frac{1}{\sqrt{Sc}}$$

$$\left(\frac{\delta_c}{\delta_u}\right)_L \approx \frac{1}{31.6}$$

→ ***Hierarchical grid method***

Flow chart of the simulation

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Hydrodynamic eq.

volume fraction eq.
$v_m^{(n)}, f^{(n)} \rightarrow f^{(n+1)}$
$\rightarrow \rho_m^{(n+1)}, \mu_m^{(n+1)}$

⇩

N.S.-eq. without pressure
$\rho_m^{(n+1)}, \mu_m^{(n+1)}, \mu_m^{(n)}, \rho_m v_m^{(n)}$
$\rightarrow \rho_m v_m(*)$

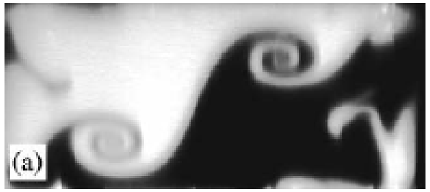
⇩

calculation of the pressure (Poisson-eq.)
$v_m(*), p^{(n)} \rightarrow p^{(n+1)}$

⇩

correction eq.
$\rho_m v_m(*), p^{(n+1)} \rightarrow v_m^{(n+1)}$

Hydrodynamic. eq. + mass transfer eq. (species)



"coarse" grid (G.G.)

- **volume fraction eq.**
- **N.S.-eq. without pressure**
- **calculation of the pressure (Poisson-eq.)**
- **correction eq.** $\rightarrow v_m^{(n+1)}$

$$\frac{\delta_c}{\delta_u} = \frac{1}{\sqrt{Sc}}$$

$$\left(\frac{\delta_c}{\delta_u}\right)_L \approx \frac{1}{31.6}$$

⇩

interpolation method
$v_m^{(n+1)}$ (G.G) $\rightarrow v_m^{(n+1)}$ (F.G)

⇩

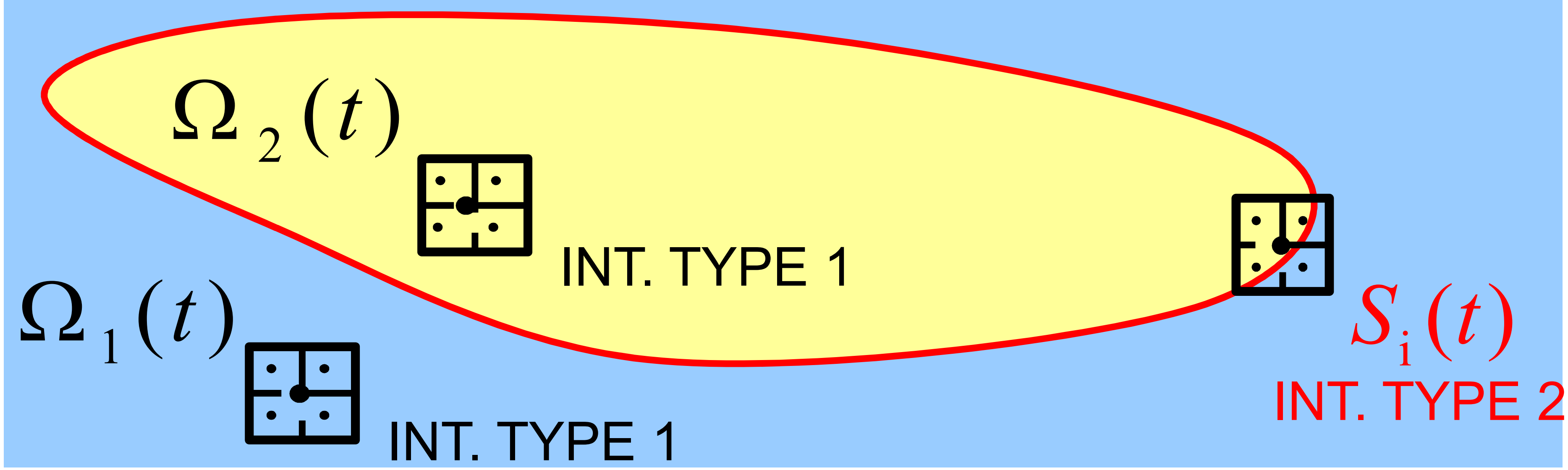
fine grid (F.G)

mass transfer eq.
$c_m^{(n)}, D_m^{(n)}, v_m^{(n+1)}$ (F.G)
$\rightarrow c_m^{(n+1)}$ (F. G.)

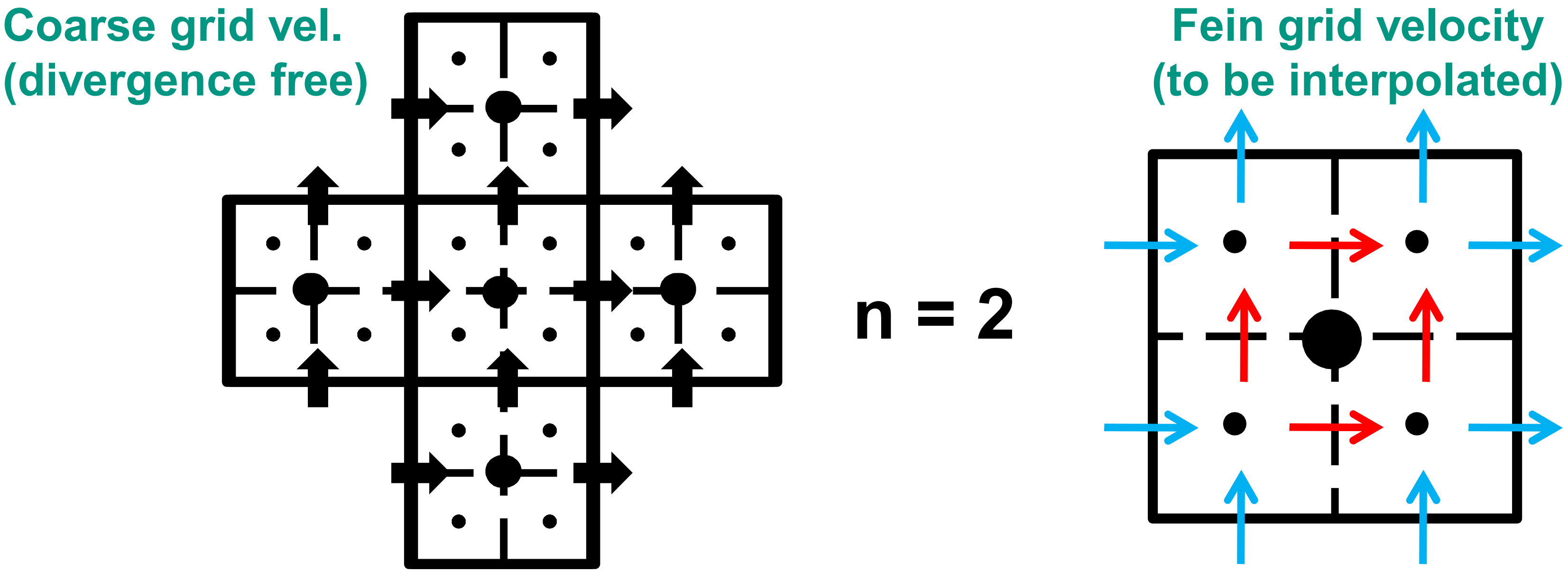
Types of algorithm

$$-\left(p_{1i}-p_{2i}\right)+\left[\mu_1\left(\nabla\mathbf{v}_1+\left(\nabla\mathbf{v}_1\right)^T\right)-\mu_2\left(\nabla\mathbf{v}_2+\left(\nabla\mathbf{v}_2\right)^T\right)\right]_i:\hat{\mathbf{n}}_1\hat{\mathbf{n}}_1=2H\ \sigma=\kappa\sigma$$

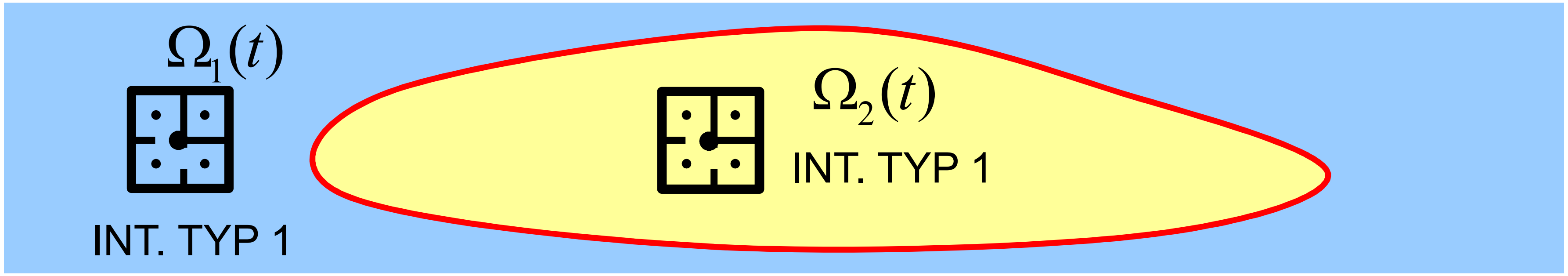
$$\left[\mu_1\left(\nabla\mathbf{v}_1+\left(\nabla\mathbf{v}_1\right)^T\right)-\mu_2\left(\nabla\mathbf{v}_2+\left(\nabla\mathbf{v}_2\right)^T\right)\right]_i:\hat{\mathbf{n}}_1\hat{t}_1=\nabla_S\sigma\ \hat{t}_1=0$$



Interpolation method (Type 1)



STEP 1: Coarse grid velocity (divergence free) → external fine grid velocites
STEP 2: external fine grid velocites → internal fine grid velocities



Interpolation algorithms

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[ScMa07] F. Schwertfirm; M. Manhart (2007).
DNS of passive-scalar transport
in turbulent channel flow at high Schmidt numbers.
Int. J. of Heat and Fluid Flow 28, 1204-1214.

-STEP1: Conservation of the mass flux and velocity gradient
-STEP2: Piecewise linear interpolation
->Not div. free (all cells) !!!

[Bals01]D. S. Balsara (2001).
Divergence-free adaptive mesh refinement
for magnetohydrodynamics (MHD).
Journal of Computational Physics 174, 614-648.

-STEP1: Piecewise linear interpolation
-STEP2: Interpolation polynomials
Complex polynomials for n>2

[LiLi04] S. Li; H. Li (2004).
A novel approach of divergence-free reconstruction
for adaptive mesh refinement.
Journal of Computational Physics 199, 1-15.

Not div. free (some cells) !!!
-STEP1: Piecewise linear interpolation
-STEP2: With help values and divergence free conditions

1-ph. flow

[Rudm98] M. Rudman(1998).
A volume-tracking method for incompressible
multifluid flows with large density variations.
Int. J. for Numerical Methods in Fluids 28, 357-378.

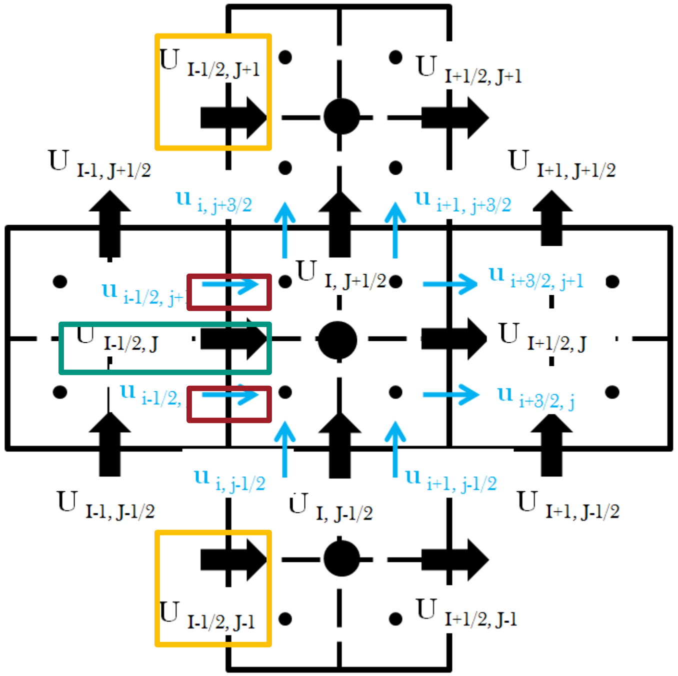
-STEP1,STEP2: Combination of piecewise linear and const. intepolation
->Div. free, but not accurated enough

[KKTr05] A. Koynov; G. Khinast; G. Tryggvason (2005).
Mass transfer and chemical reactions
in bubble swarms with dynamics interfaces.
AIChE Journal 51 (10), 2786-2800.

Not div. free (some cells) !!!
-STEP1: Piecewise linear interpolation
-STEP2: Interpolation of vel. grad. from the coarse to the fine grid

2-ph. flow

STEP1 Interpolation [ScMa07]



$$
\begin{bmatrix} u_{i-\frac{1}{2},j+1} \\ u_{i-\frac{1}{2},j} \\ u_{i+\frac{3}{2},j+1} \\ u_{i+\frac{3}{2},j} \\ u_{i,j-\frac{1}{2}} \\ u_{i+1,j-\frac{1}{2}} \\ u_{i,j+\frac{3}{2}} \\ u_{i+1,j+\frac{3}{2}} \end{bmatrix}
=
\begin{bmatrix}
1 & +1/8 & -1/8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -1/8 & +1/8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & +1/8 & -1/8 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & -1/8 & +1/8 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & +1/8 & -1/8 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & -1/8 & +1/8 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & +1/8 & -1/8 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1/8 & +1/8
\end{bmatrix}
\begin{bmatrix} U_{I-\frac{1}{2},J} \\ U_{I-\frac{1}{2},J+1} \\ U_{I-\frac{1}{2},J-1} \\ U_{I+\frac{1}{2},J} \\ U_{I+\frac{1}{2},J+1} \\ U_{I+\frac{1}{2},J-1} \\ U_{I,J-\frac{1}{2}} \\ U_{I-1,J-\frac{1}{2}} \\ U_{I+1,J-\frac{1}{2}} \\ U_{I,J+\frac{1}{2}} \\ U_{I-1,J+\frac{1}{2}} \\ U_{I+1,J+\frac{1}{2}} \end{bmatrix}
$$

Cons. of mass flux on the surface

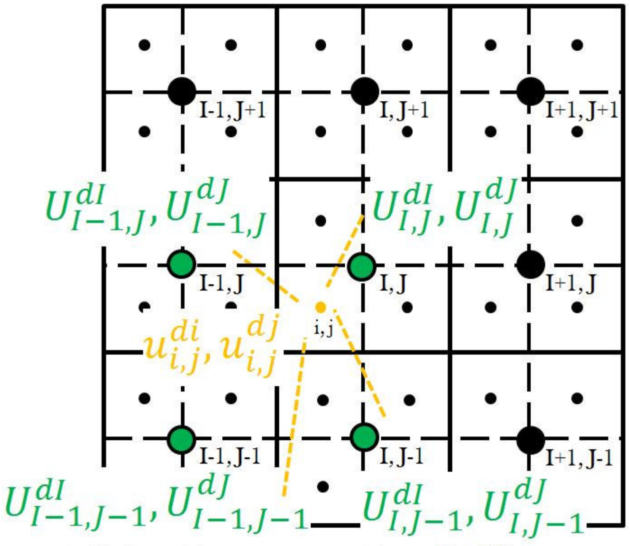
$$U_{I-\frac{1}{2},J} \cdot (\Delta_J) = u_{i-\frac{1}{2},j+1} \cdot (\delta_{j+1}) + u_{i-\frac{1}{2},j} \cdot (\delta_j)$$

Gradient approach

$$\frac{U_{I-\frac{1}{2},J+1} - U_{I-\frac{1}{2},J-1}}{\Delta_{J+1}/2 + \Delta_J + \Delta_{J-1}/2} = \frac{2 \cdot \left(u_{i-\frac{1}{2},j+1} - u_{i-\frac{1}{2},j}\right)}{\delta_{j+1} + \delta_j}$$

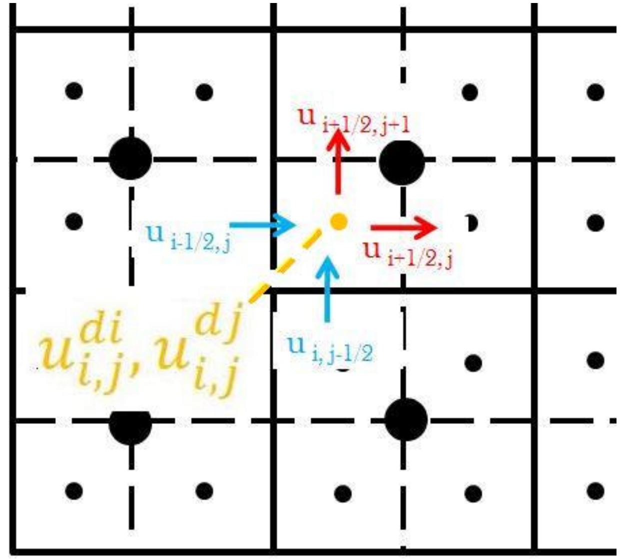
[ScMa07] F. Schwertfirm; M. Manhart (2007). DNS of passive-scalar transport in turbulent channel flow at high Schmidt numbers. International Journal of Heat and Fluid Flow 28, 1204-1214.

STEP2 interpolation [KKTr05]



Interpolation of the velocity gradient

$$u^{di}_{i,j} \qquad u^{dj}_{i,j}$$



Gradient approach

$$u^{di}_{i,j} = \frac{u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}}{\delta_i}$$

$$u^{dj}_{i,j} = \frac{u_{i,j+\frac{1}{2}} - u_{i,j-\frac{1}{2}}}{\delta_j}$$

[KKTr05]A. Koynov; G. Khinast; G. Tryggvason (2005).
Mass transfer and chemical reactions in bubble swarms with dynamics interfaces.
AIChE Journal 51 (10), 2786-2800.

Interpolation method (Type 1)

-**STEP1**:
- -Cons. of the massflux
- -Cons. velocity gradient

-**STEP2**:
- a) Interpolation of vel. gradient from the coarse to the fine grid
- b) Use of gradient approach
- c) Divergence free condition

Unknow velocities (STEP1):

$$st1 = n^{(DIM-1)} 2 \; (DIM)$$

Unknow velocites (STEP2):

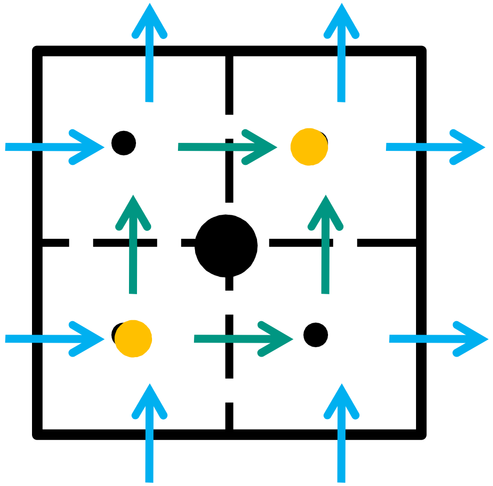
$$st2 = n^{(DIM-1)} (n-1) \; (DIM)$$

n=2

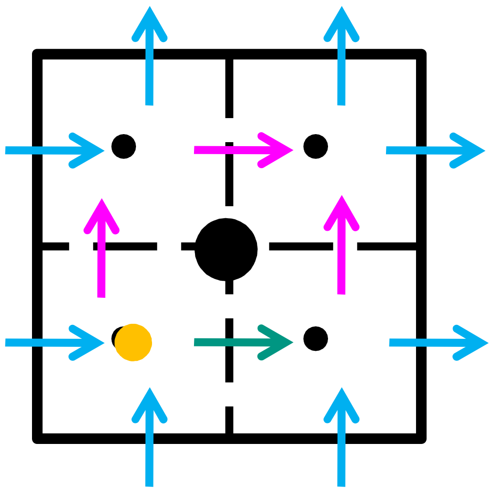
st1=4x2=8

st2=4

Exp: 2D, n = 2



Not div. free in all cells !!!



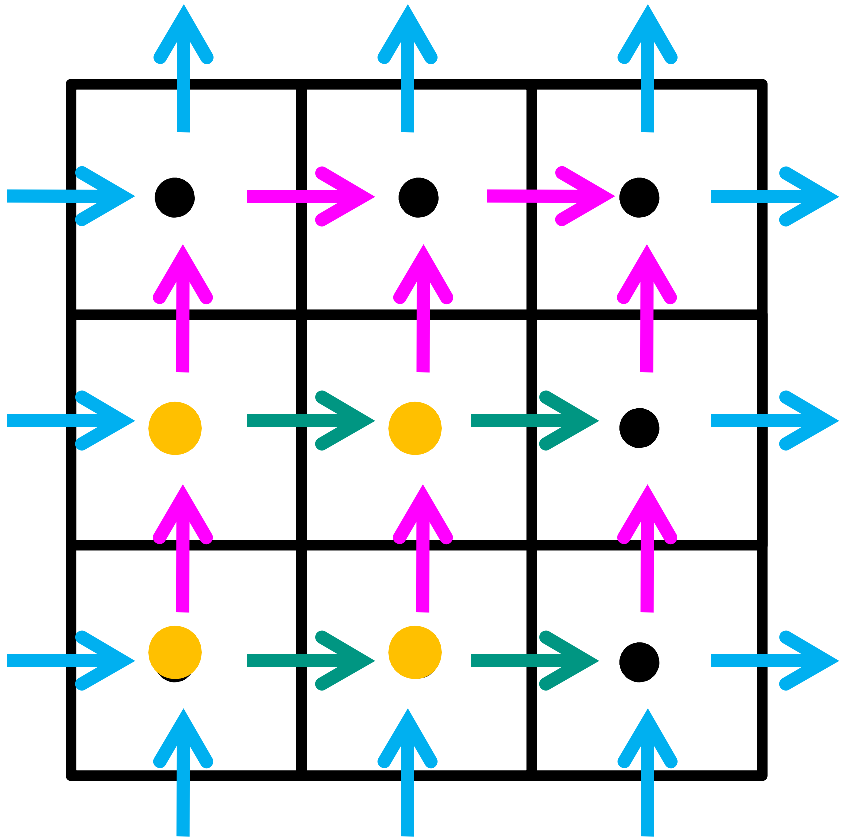
Div. free cond. in all cells !!!

Interpolation method (Type 1)

Exp: 2D, n = 3

-**STEP1**:
- -Cons. of the massflux
- -Cons. velocity gradient

-**STEP2**:
- a) Interpolation of vel. gradient from the coarse to the fine grid
- b) Use of gradient approach
- c) Divergence free condition



Unknow velocities (STEP1):

$$st1 = n^{(DIM-1)} 2\ (DIM)$$

Unknow velocites (STEP2):

$$st2 = n^{(DIM-1)} (n-1)\ (DIM)$$

n=3

st1=4x3=12

st2=12

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OUTLOOK

- Divergence free velocity interpolation
  - 2D, Refinement factor n=2 (Type 1) ✓
  - 2D, Refinement factor n>2 (Type1) ✓ **(Test phase)**
  - 2D, Refinement factor n>2 (Type 2)
  - 3D, Refinement factor n>2 (Type 1,Type 2)
- Single field mass transfer eq.
  - Better discretization of additional Term
- Method implementation (TURBIT-VOF)
- Validation for mass transfer
  - Taylor flow