Implementation and Validation of Wall Slip Velocity and Temperature Jump Boundary Conditions for Gas Flow in Microdevices

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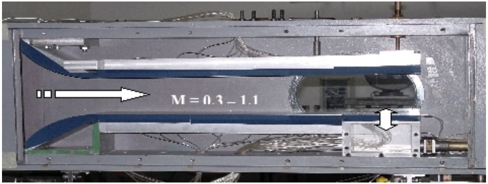
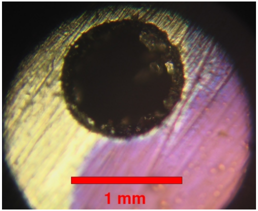
Objective

Use *Navier Stokes* Flow Solver for Microdevices

Flow in drilled holes on airfoil



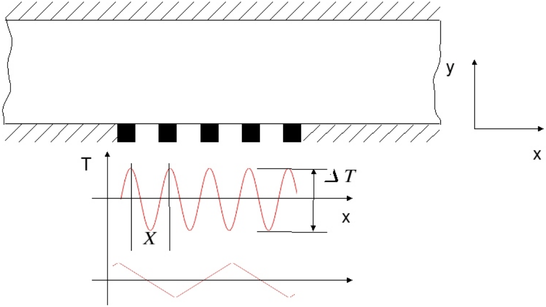


IMP PAN
Institute of Fluid Flow Machinery
Gdańsk
Prof. Doerffer

Objective

Use *Navier Stokes* Flow Solver for Microdevices

- Cooling of microfluidic devices



Outline

Knudsen Number

Mean free path λ

Definition

$$\lambda = \frac{k \cdot T}{\sqrt{2} \cdot \pi \cdot d^2 \cdot p}$$

$k \ldots$ Boltzmann constant
$d \ldots$ Molecular diameter

Knudsen number Kn

Classification of flows

$$Kn = \frac{\lambda}{L}$$

$L \ldots$ Length scale

Alternative length scale expression

$$L = \frac{\rho}{\left|\frac{\partial \rho}{\partial y}\right|}$$

Knudsen Number

Mean free path λ

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Knudsen number *Kn*

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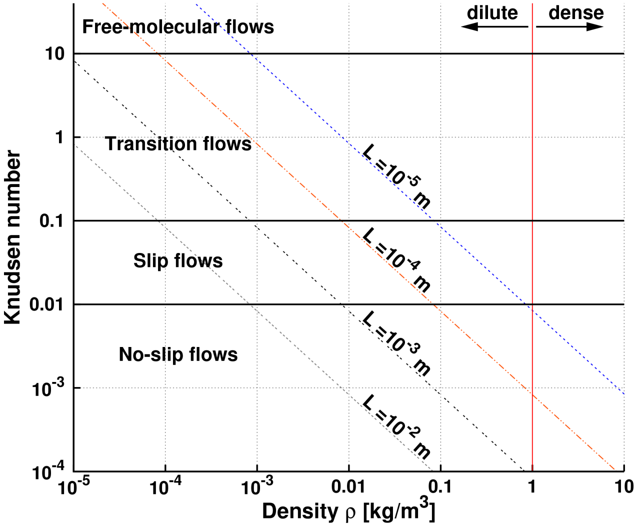
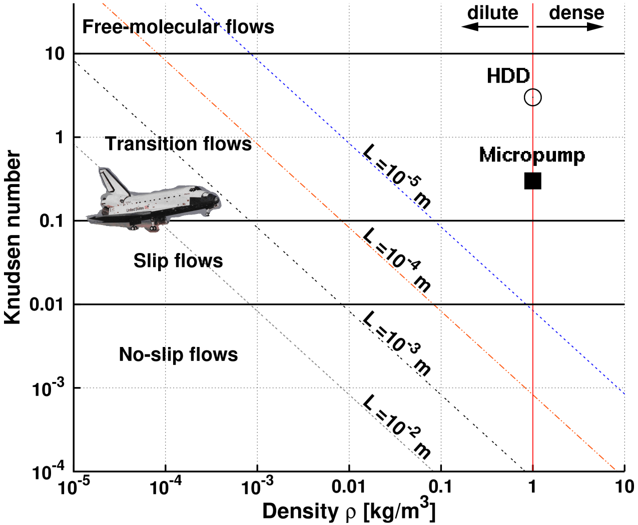
Air Flows - Classification



Air Flows - Classification



Maxwell Slip Velocity Condition

Equation

$$u_{fluid} - u_{wall} = \frac{2-\sigma_V}{\sigma_V}\lambda\frac{\partial u}{\partial y} + \frac{3}{4}\frac{\mu}{\rho T}\frac{\partial T}{\partial x}$$

Symbols

σ_V... Tangential momentum accommodation coefficient (TMAC)

Maxwell, J.C. (1879)

Maxwell Slip Velocity Condition

Equation

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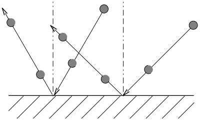
Tangential Momentum Accommodation Coefficient σ_V



- $\sigma_V = \dfrac{\text{particles contributing streamwise momentum}}{\text{total number of impinging particles}}$
- $\sigma_V = 1$ - diffuse reflection of particles
- $\sigma_V < 1$ - diffuse/specular reflection

Experimental observations:

$\sigma_V \approx 0.2$	$\sigma_V \approx 0.65 \ldots 0.96$	$\sigma_V \approx 0.75 \ldots 1$
Molecular beams on metal-coated surfaces	He, Ar, Kr on titanium-coated surfaces	Ar, N_2, CO_2 in silicon micro-channels
Steinheil et al. (1977)	Nakarjakov et al. (1994)	Arkilic (1997)

Smoluchowski Temperature Jump

Equation

$$T_{fluid} - T_{wall} = \frac{2-\sigma_T}{\sigma_T} \frac{2\gamma}{\gamma+1} \frac{\lambda}{Pr} \frac{\partial T}{\partial y}$$

$$Pr = \frac{\mu \cdot c_p}{k_L}$$

Symbols

$\sigma_T \ldots$ Thermal accommodation coefficient
$\gamma \ldots$ Specific heat ratio
$c_p \ldots$ Specific heat
$k_L \ldots$ Thermal conductivity

Smoluchowski, M. (1898)

Higher Order Expansion

Expansion

- Slip velocity, temperature gradient neglected:

$$u_{fluid} - u_{wall} = \frac{2-\sigma_V}{\sigma_V}\left[\lambda\frac{\partial u}{\partial y} + \frac{\lambda^2}{2}\frac{\partial^2 u}{\partial y^2} + \frac{\lambda^3}{6}\frac{\partial^3 u}{\partial y^3}\dots\right]$$

- Temperature jump:

$$T_{fluid} - T_{wall} = \frac{2-\sigma_T}{\sigma_T}\frac{2\gamma}{\gamma+1}\frac{1}{Pr}\left[\lambda\frac{\partial T}{\partial y} + \frac{\lambda^2}{2}\frac{\partial^2 T}{\partial y^2} + \frac{\lambda^3}{6}\frac{\partial^3 T}{\partial y^3}\dots\right]$$

- Generally higher order expressions not applied with *Navier Stokes* equations approach

Extended Slip Velocity Formulation

Curved surface influence

$$u_{fluid} - u_{wall} = \frac{2-\sigma_v}{\sigma_v}\lambda\left[\frac{\partial u}{\partial y} + \frac{\partial u}{\partial x} + \frac{\mu}{\rho}\left(\frac{1}{\rho}\frac{\partial^2 \rho}{\partial x \partial y} - \frac{1}{T}\frac{\partial^2 T}{\partial x \partial y}\right)\right] + \frac{3}{4}\frac{\mu}{\rho T}\frac{\partial T}{\partial x}$$

Thermal Stress Slip Flow Term

$$\frac{2-\sigma_v}{\sigma_v}\lambda\left[\frac{\mu}{\rho}\left(-\frac{1}{T}\frac{\partial^2 T}{\partial x \partial y}\right)\right]$$

Lockerby, D.A., Reese, J.M., Emerson, D.R., Barber, R.W. (2004)

Sone, Y. (2000)

Extended Slip Velocity Formulation

Curved surface influence

$$
\begin{aligned}
u_{fluid} - u_{wall} \quad = \quad & \frac{2-\sigma_V}{\sigma_V}\lambda\left[\frac{\partial u}{\partial y} + \frac{\partial u}{\partial x} + \right. \\
& \left. \frac{\mu}{\rho}\left(\frac{1}{\rho}\frac{\partial^2 \rho}{\partial x \partial y} - \frac{1}{T}\frac{\partial^2 T}{\partial x \partial y}\right)\right] + \frac{3}{4}\frac{\mu}{\rho T}\frac{\partial T}{\partial x}
\end{aligned}
$$

Thermal Stress Slip Flow Term

$$
\frac{2-\sigma_V}{\sigma_V}\lambda\left[\frac{\mu}{\rho}\left(-\frac{1}{T}\frac{\partial^2 T}{\partial x \partial y}\right)\right]
$$

Lockerby, D.A., Reese, J.M., Emerson, D.R., Barber, R.W. (2004)
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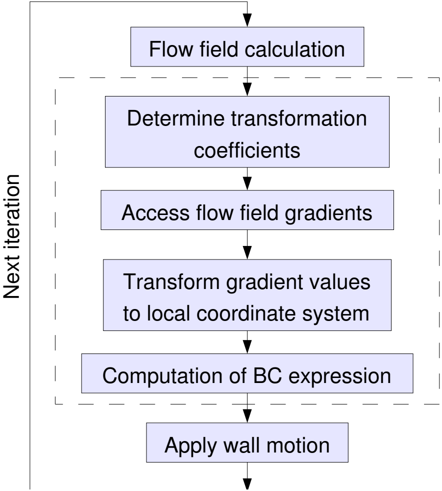
Schematic Algorithm



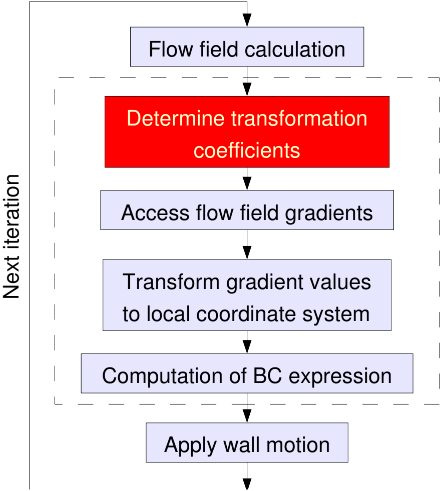
```
        .
ND_SET(F_UDMI(face,f_thread,0),
  F_UDMI(face,f_thread,1),
  F_UDMI(face,f_thread,2),
  NVD_DOT(u,1,0,0)/a,...
        .

        .
tangential_slip=NVD_DOT(Coeff1,
  NV_DOT(Coeff1,C_U_G(cell,c_thread)),
  NV_DOT(Coeff1,C_V_G(cell,c_thread)),
  NV_DOT(Coeff1,C_W_G(cell,c_thread))) ;
normal_slip=   NVD_DOT(Coeff1,
  NV_DOT(Coeff2,C_U_G(cell,c_thread)),
  NV_DOT(Coeff2,C_V_G(cell,c_thread)),
  NV_DOT(Coeff2,C_W_G(cell,c_thread))) ;
        .

        .
slip = ((2-TMAC)/TMAC) * MeanFreePath *
  (tangential_slip+normal_slip) ;
        .

        .
#ifdef   WALLMOTION
  dveloc= F_UDSI(face,f_thread,1) + slip...
#else
  dveloc= slip + thcreep;
#endif
        .
```

Schematic Algorithm



Next iteration

Flow field calculation

Determine transformation coefficients

Access flow field gradients

Transform gradient values to local coordinate system

Computation of BC expression

Apply wall motion

```
      .
ND_SET(F_UDMI(face,f_thread,0),
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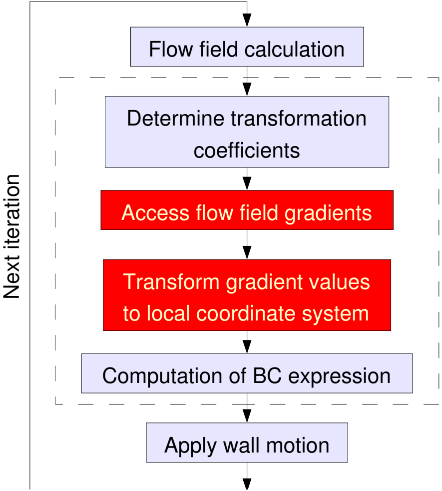
Schematic Algorithm



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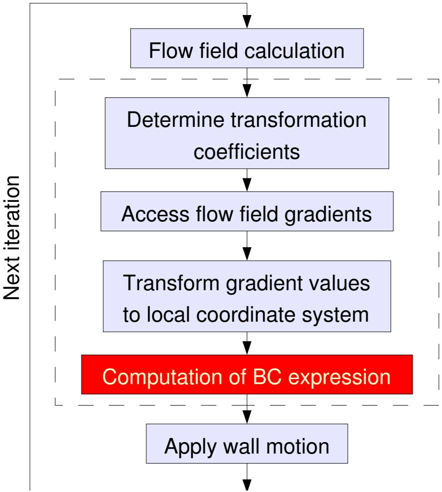
Schematic Algorithm



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#else
  dveloc= slip + thcreep;
#endif
        .
```
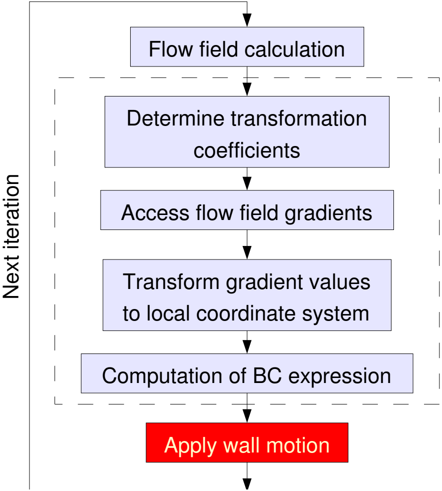

Schematic Algorithm



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slip = ((2-TMAC)/TMAC) * MeanFreePath *
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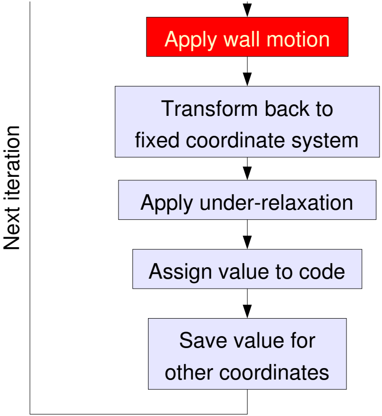
#ifdef   WALLMOTION
  dveloc= F_UDSI(face,f_thread,1) + slip...
#else
  dveloc= slip + thcreep;
#endif
      .
```

Schematic Algorithm (contd.)



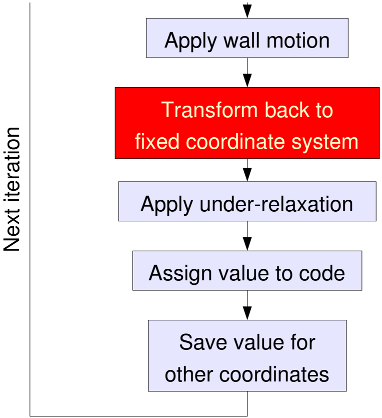
```
        .
dveloc *= Coeff1[0];
        .

        .
#ifdef  UNDERRLX
  dveloc = (1-UDRLXCOEFF) * u[0] +
           UDRLXCOEFF  * dveloc;
#endif
        .

        .
F_PROFILE(face,f_thread,index) = dveloc;
        .

        .
C_UDMI(cell,c_thread,6) = dveloc;
C_UDMI(cell,c_thread,7) = normal_slip;
        .
```

Schematic Algorithm (contd.)



Apply wall motion

Transform back to fixed coordinate system

Apply under-relaxation

Assign value to code

Save value for other coordinates

```
        .
dveloc *= Coeff1[0];
        .

        .
#ifdef   UNDERRLX
  dveloc = (1-UDRLXCOEFF) * u[0] +
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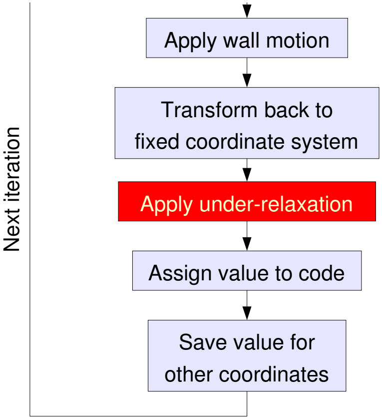
        .

        .
C_UDMI(cell,c_thread,6) = dveloc;
C_UDMI(cell,c_thread,7) = normal_slip;
        .
```

Schematic Algorithm (contd.)



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        .
dveloc *= Coeff1[0];
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#ifdef   UNDERRLX
  dveloc = (1-UDRLXCOEFF) * u[0] +
             UDRLXCOEFF  * dveloc;
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F_PROFILE(face,f_thread,index) = dveloc;
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C_UDMI(cell,c_thread,6) = dveloc;
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        .
```
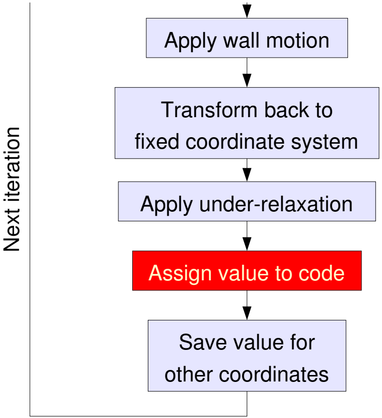

Schematic Algorithm (contd.)



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             UDRLXCOEFF  * dveloc;
#endif
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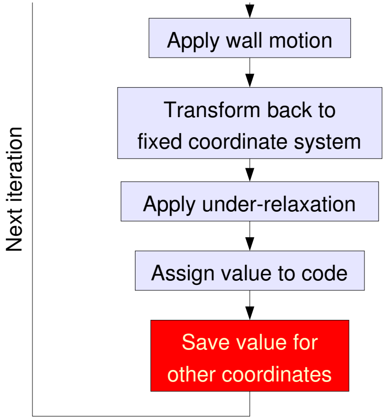
F_PROFILE(face,f_thread,index) = dveloc;
       .

       .
C_UDMI(cell,c_thread,6) = dveloc;
C_UDMI(cell,c_thread,7) = normal_slip;
       .
```

Schematic Algorithm (contd.)



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        .
dveloc *= Coeff1[0];
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        .
#ifdef   UNDERRLX
  dveloc = (1-UDRLXCOEFF) * u[0] +
               UDRLXCOEFF  * dveloc;
#endif
        .

        .
F_PROFILE(face,f_thread,index) = dveloc;
        .

        .
C_UDMI(cell,c_thread,6) = dveloc;
C_UDMI(cell,c_thread,7) = normal_slip;
        .
```
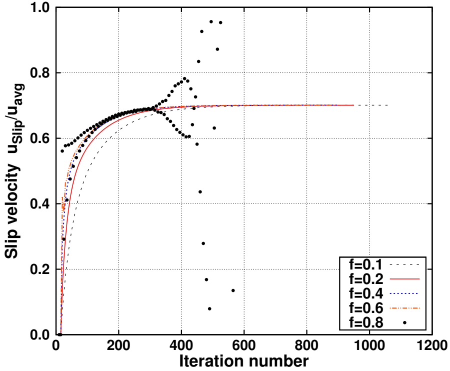
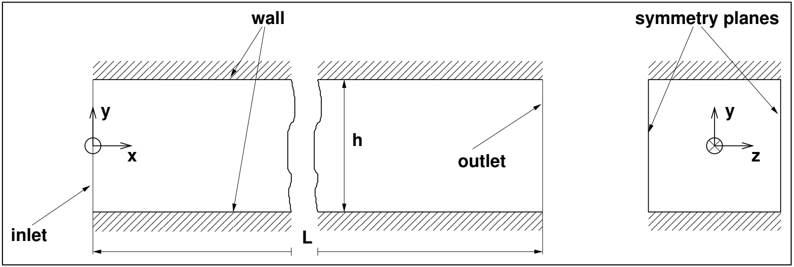

Under-relaxation factor *f*



- Application of under-relaxation:
  $u_k^n = (1-f)\cdot u_k^{n-1} + f\cdot u_k'^n$
- Case here - starting from initial guess
- Leading to final solution for most *f* values

Test Cases - Outline

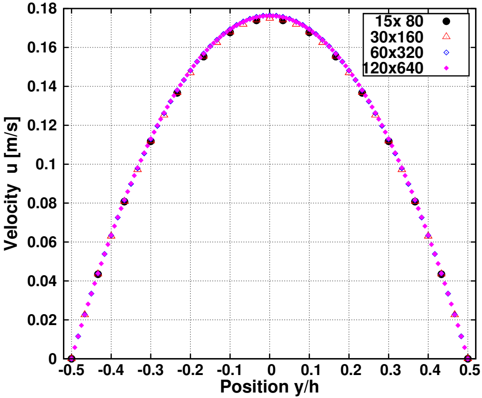
Test Case 1 - Setup and Boundary Conditions



- Laminar two-dimensional setup
- Ideal gas: air
- $h = 10^{-7} \dots 10^{-3} m$ (no-slip and slip flow regimes)
- Static pressure difference between inlet and outlet planes $\Delta p = 5\ Pa$
- *Slip velocity condition* applied at walls

Test Case 1 - Setup

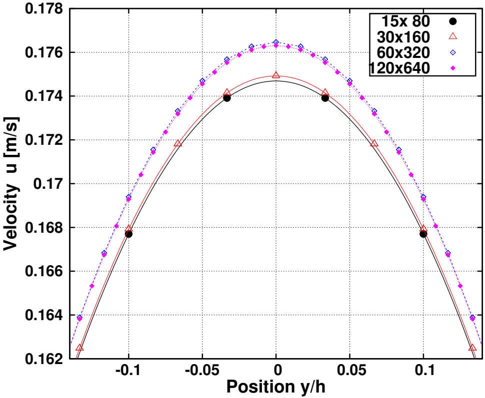
Grid Information



- Initial set of grids for no-slip flow tested
- Chosen grids are:
  - 25x125x1
  - 50x250x1
  - 100x500x1

Test Case 1 - Setup

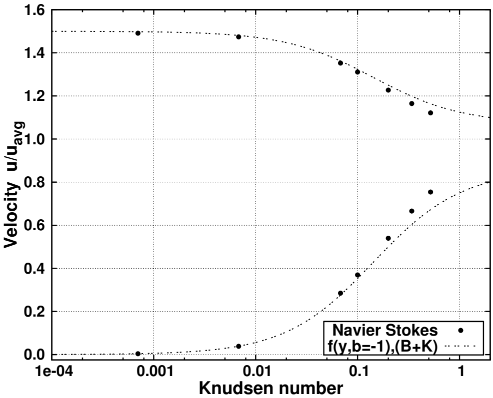
Grid Information



- Initial set of grids for no-slip flow tested
- Chosen grids are:
    - 25x125x1
    - 50x250x1
    - 100x500x1

Test Case 1 - Result

Knudsen Number versus Velocities



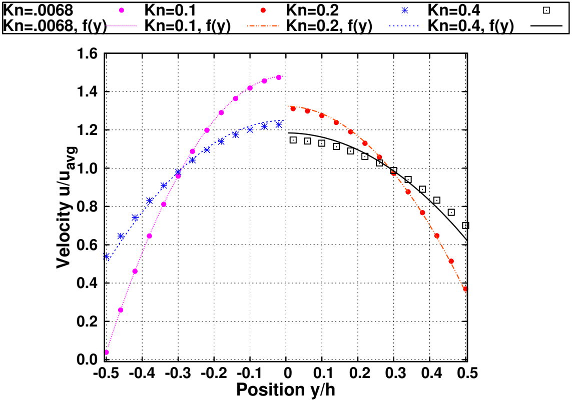
- Good agreement with reference(curve) up to $Kn \approx 0.1$

$$\frac{u(Kn,y)}{u_{avg}} = \frac{-(y/h)^2+y/h+\frac{Kn}{1-bKn}}{1/6+\frac{Kn}{1-bKn}}$$

Beskok, A., Karniadakis, G. E. (1999)

Test Case 1 - Result

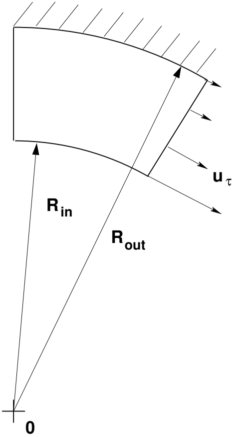
Channel Velocity Profiles



- Good agreement with reference(curves) up to $Kn \approx 0.1$

Beskok, A., Karniadakis, G. E. (1999)

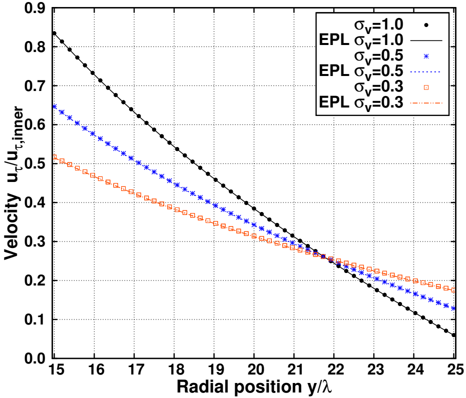
Test Case 2 - Setup and Boundary Conditions



- Laminar two-dimensional setup, symmetry planes in depth direction
- Periodicity in circumferential direction
- Ideal gas: air
- $R_{out} = 25\ \lambda$, $R_{in} = 15\ \lambda$, $\lambda(T = 300\ K) = 6.9 \cdot 10^{-7} m$
- *Slip velocity condition* with wall motion applied

Test Case 2 - Result

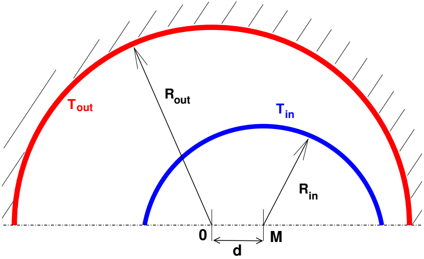
Radial Velocity distribution



- Radial position given as a multiple of mean free path λ
- Good agreement with analytical approach(curves)

Einzel, D., Panzer, P., Liu, M. (1990) [EPL]

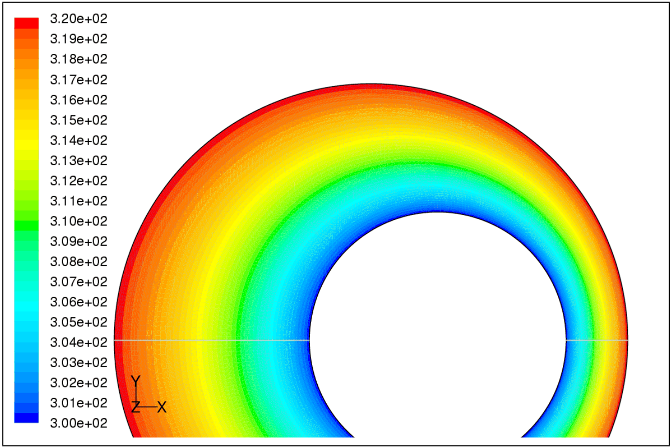
Test Case 3 - Setup and Boundary Conditions



- Two-dimensional setup, symmetry planes present
- Laminar case; ideal gas: air
- Temperature at walls: $T_{in} = 300\ K$, $T_{out} = 320\ K$
- $R_{out}/R_{in} = 2$, $R_{out} = 5 \cdot 10^{-4} m$, $d = 1.3 \cdot 10^{-4} m$
- *Extended slip velocity condition* and *temperature jump* applied at walls

Test Case 3 - Result

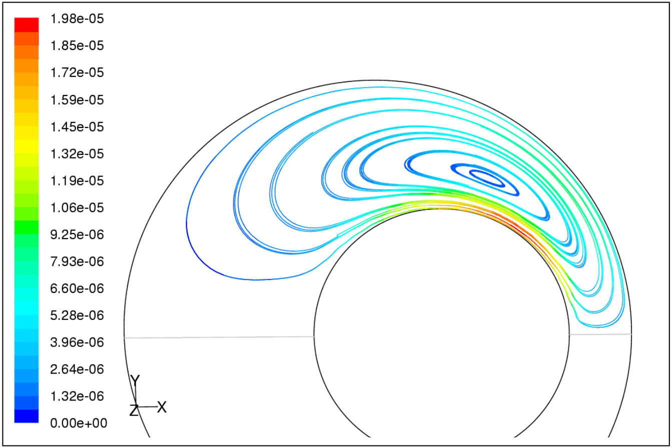
Temperature Field



- Values indicate temperature in [K]
- Upper part of domain shown

Test Case 3 - Result

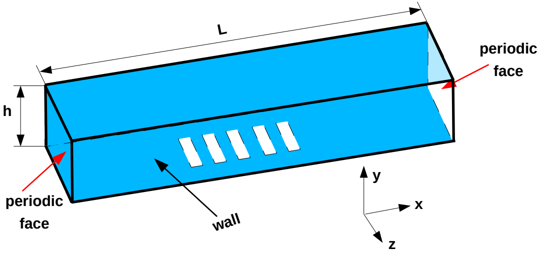
Path Lines



- Values indicate velocity magnitude in [m/s]
- Upper part of domain shown

Chip Cooling - Setup and Boundary Conditions

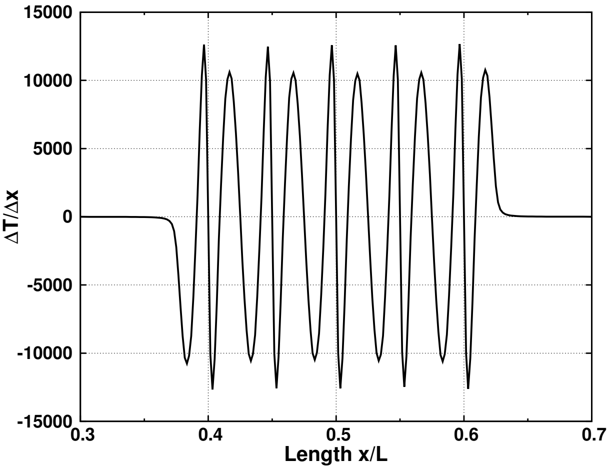
Domain



- Threedimensional laminar case, ideal gas: air
- Height h and depth 10^{-4} m, length $L = 2 \cdot 10^{-3}$ m
- Periodic pair inlet/outlet, pressure gradient 9 [Pa/m]
- *Slip velocity condition* and *temperature jump* conditions at lower y wall, T=300 K
- Temperature at plates 300 ± 1 K
- Other faces are symmetry planes

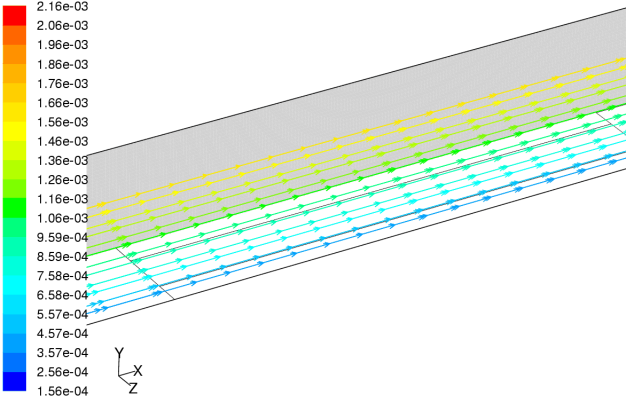
Chip Cooling - Result

Temperature Gradient vs Length



Chip Cooling - Result

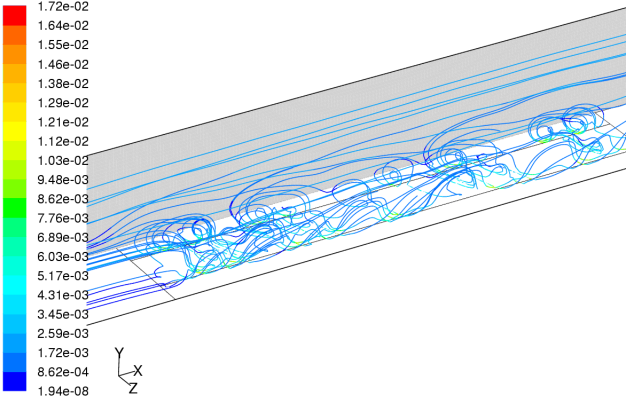
Path Lines for No-Slip Flow



- Colour indicates velocity magnitude in [m/s]

Chip Cooling - Result

Path Lines for Slip Flow



- Colour indicates velocity magnitude in [m/s]

Summary

- Boundary conditions for slip velocity and temperature jump implemented into finite volume fluid dynamics solver
- Validation of implemented routines performed
- Chip cooling application can be modelled

References

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