Finite Element Simulation of Particle-Laden Gas Flows with Application to the Arc Spraying Process

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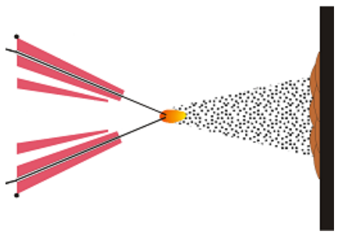
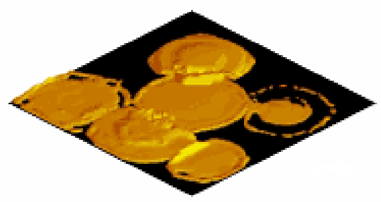
Contents & Aims

Aims

- Numerical simulation of the compressible particle-laden gas flow between the nozzle and the substrate
- Macroscopic 2-fluid model
- Development of implicit high-resolution finite element TVD-schemes based on algebraic flux correction





Contents

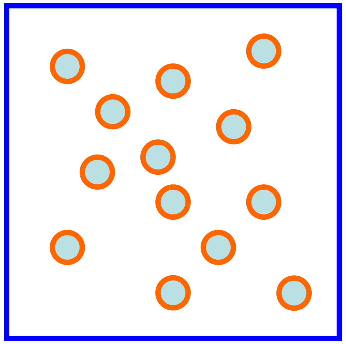
- Modelling
- FEM discretization of the Euler equations
- FEM discretization of the non-hyperbolic dust equations
- Benchmarking

Modelling

Main assumptions

- Continuum description of both phases
- Conservation of mass, momentum, and energy
- Coupling via the drag force and heat exchange
- Dilute flow (small volume fraction of particles)
- Pressureless particlulate phase, ideal gas
- No particle collisions occur

Control volume



Interphase terms

$$F_D = \alpha_p \gamma_D (u_p - u_g)$$

$$Q_T = \alpha_p \gamma_T (T_p - T_g)$$

The 2-Fluid Model

Gas phase:

$$\begin{aligned}
\partial_t(\alpha_g\rho_g)+\nabla\cdot(\alpha_g\rho_g u_g) &= 0\\
\partial_t(\alpha_g\rho_g u_g)+\nabla\cdot(\alpha_g\rho_g u_g\otimes u_g+\alpha_g PI) &= P\nabla\alpha_g+F_D\\
\partial_t(\alpha_g\rho_g E_g)+\nabla\cdot(\alpha_g u_g(\rho_g E_g+P)) &= PV_i\nabla\alpha_g+V_i\cdot F_D+Q_T
\end{aligned}$$

Particulate phase:

$$\begin{aligned}
\partial_t(\alpha_p\rho_p)+\nabla\cdot(\alpha_p\rho_p u_p) &= 0\\
\partial_t(\alpha_p\rho_p u_p)+\nabla\cdot(\alpha_p\rho_p u_p\otimes u_p) &= P\nabla\alpha_p-F_D\\
\partial_t(\alpha_p\rho_p E_p)+\nabla\cdot(\alpha_p u_p\rho_p E_p) &= PV_i\nabla\alpha_p-V_i\cdot F_D-Q_T
\end{aligned}$$

Saturation condition: $\alpha_g+\alpha_p=1$

- Two-way coupling via the volume fractions and interphase transfer terms.

Operator-Splitting

$$\partial_t \begin{bmatrix} U_g \\ U_p \end{bmatrix} + \nabla \cdot \begin{bmatrix} F_g \\ F_p \end{bmatrix} = \begin{bmatrix} S_g \\ S_p \end{bmatrix}$$

1. Hyperbolic step

$$\begin{aligned} \frac{U_g^{n+1/2} - U_g^n}{\Delta t} + \nabla \cdot F_g^{n+1/2} &= 0 \\ \frac{U_p^{n+1/2} - U_p^n}{\Delta t} + \nabla \cdot F_p^{n+1/2} &= 0 \end{aligned}$$

Hyperbolic equations

2. Source term step

$$\begin{aligned} \frac{U_g^{n+1} - U_g^{n+1/2}}{\Delta t} &= S_g^{n+1} \\ \frac{U_p^{n+1} - U_p^{n+1/2}}{\Delta t} &= S_p^{n+1} \end{aligned}$$

Nodal ODEs

Discretization of Convective Terms

High-order scheme:

$$M_C \frac{dU}{dt} = KU$$

Low-order scheme:

$$M_L \frac{dU}{dt} = KU + DU = LU$$

High-resolution scheme:

$$M_L \frac{dU}{dt} = KU + DU + F^* U = K^* U$$

Equivalent representation:

$$M_L \frac{dU}{dt} = L^* U$$

Euler Equations: High-Order Scheme

Galerkin FEM:

$$\sum_j m_{ij} \frac{dU_j}{dt} = -\sum_j c_{ij} \cdot F_j, \quad \forall i$$

Matrix coefficients:

$$m_{ij} = \int_\Omega \varphi_i \varphi_j dx \qquad c_{ij} = \int_\Omega \varphi_i \nabla \varphi_j dx$$

Lumped mass Galerkin scheme:

$$m_i = \sum_j m_{ij} \quad \Rightarrow \quad m_i \frac{dU_i}{dt} = -\sum_j c_{ij} \cdot F_j, \quad \forall i$$

$$F(U) = A(U)U \quad \Rightarrow \quad M_L \frac{dU}{dt} = KU$$

Low-Order Scheme: Edge-Based Decomposition

Characteristic LED criterion:

A semi-discrete scheme of the form $m_i \frac{dU_i}{dt} = \sum_{j \neq i} L_{ij} \left(U_j - U_i \right)$

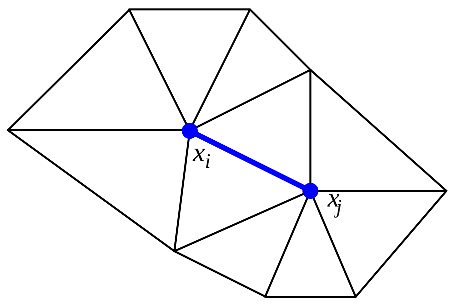
is LED, if all off-diagonal blocks L_{ij} are positive semi-definite.

$$
\begin{aligned}
(KU)_i &= -\sum_j c_{ij} \cdot F_j \\
&= -\sum_{j \neq i} c_{ij} \cdot \left(F_j - F_i \right)
\end{aligned}
$$

$$
\begin{aligned}
(KU)_i &= -\sum_{j \neq i} c_{ij}^{(x)} \left(F_j^{(x)} - F_i^{(x)} \right) + c_{ij}^{(y)} \left(F_j^{(y)} - F_i^{(y)} \right) \\
&= -\sum_{j \neq i} \left(c_{ij}^{(x)} A_{ij}^{(x)} + c_{ij}^{(y)} A_{ij}^{(y)} \right) \left(U_j - U_i \right)
\end{aligned}
$$

Roe linearization

$$F_j^{(x,y)} - F_i^{(x,y)} = A_{ij}^{(x,y)} \left(U_j - U_i \right)$$



Design of the Artificial Diffusion Operator

Requirements:

- Block symmetry, zero row and column sums
- Enough dissipation to enforce the LED criterion

Local diffusion operator: $D_{loc} = \begin{pmatrix} -D_{ij} & D_{ij} \\ D_{ij} & -D_{ij} \end{pmatrix}$, $\quad D_{ij} = R_{ij} \left| \Lambda_{ij} \right| R_{ij}^{-1}$

Diffusive fluxes: $f_{ij}^{diff} = D_{ij} \left(U_j - U_i \right)$, $\quad f_{ji}^{diff} = -f_{ij}^{diff}$

Low-order operator: $L_{ij} = K_{ij} + D_{ij} = R_{ij} \Lambda_{ij} R_{ij}^{-1} + R_{ij} \left| \Lambda_{ij} \right| R_{ij}^{-1}$

Flux Limiting & Characteristic Variables

Characteristic variables: $\frac{\partial U}{\partial t} + A^d \frac{\partial U}{\partial x^d} = 0$ $\xrightarrow[A^d = R \Lambda R^{-1}]{W = R^{-1} U}$ $\frac{\partial W_k}{\partial t} + \lambda_k^d \frac{\partial W_k}{\partial x^d} = 0$

Compute characteristic variables for each space dimension separately

- Decoupling of the linearized Euler equations along the edge ij
- Characteristic flux limiter of TVD type (Kuzmin 2007)

$$\Delta W_{ij} = R_{ij}^{-1}\left(U_j - U_i\right) \quad \Longrightarrow \quad F_{ij}^* = R_{ij}\Delta \hat{W}_{ij} \qquad F_{ji}^* = -F_{ij}^*$$

High-resolution scheme: $\left(K^* U\right)_i = \sum_{j \neq i}\left(K_{ij} + D_{ij} - F_{ij}^*\right)\left(U_j - U_i\right)$

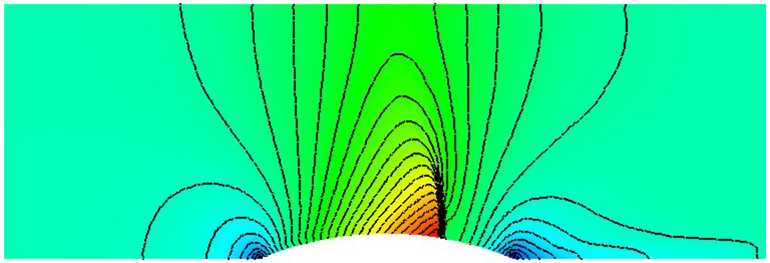
Weak Boundary Conditions: Euler Equations

Integration by parts:

$$\sum_j \int_\Omega \varphi_i \varphi_j dx \frac{dU_j}{dt} = \sum_j \int_\Omega \varphi_j \nabla \varphi_i dx \cdot F_j - \sum_j \int_{\partial\Omega} \varphi_i \varphi_j n ds \cdot F_j, \quad \forall i$$

- Improved convergence rates and robustness in steady computations
- Exclusively the boundary integrals are affected by the boundary conditions
- Fully implicit boundary treatment

Transonic Ni-Bump



$$\sum_j \int_{\partial\Omega} \varphi_i \varphi_j n ds \cdot F_j \quad \Rightarrow \quad \boxed{\text{Overwrite the boundary flux by the imposed boundary condition}} \quad \Rightarrow \quad \sum_j \int_{\partial\Omega} \varphi_i \varphi_j n ds \cdot \tilde{F}_j$$

Dust Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \begin{pmatrix} u \\ v \end{pmatrix} \right) = 0$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot \left(\rho u \begin{pmatrix} u \\ v \end{pmatrix} \right) = 0$$

$$\frac{\partial \rho v}{\partial t} + \nabla \cdot \left(\rho v \begin{pmatrix} u \\ v \end{pmatrix} \right) = 0$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left(\rho E \begin{pmatrix} u \\ v \end{pmatrix} \right) = 0$$

- The dust equations lack hyperbolicity
- Transformation to characteristic variables neither possible nor necessary
- Scalar dissipation, modified Rusanov's flux
- Flux limiting in terms of conservative variables

Discrete transport operator: $$k_{ij} = -c_{ij} \cdot \begin{pmatrix} u_j \\ v_j \end{pmatrix}$$

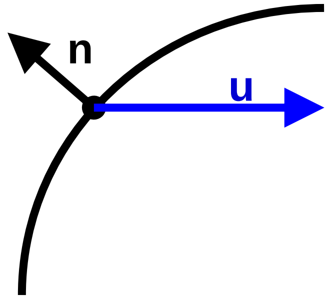
Scalar LED criterion: $$d_{ij} = d_{ji} = \max\{0, -k_{ij}, -k_{ji}\}$$ → Insufficient amount of diffusion to capture the whole solution

Modified Rusanov: $$d_{ij} = d_{ji} = \max\{|k_{ij}|, |k_{ji}|\}$$ → Sufficient amount of diffusion to compute a physical solution

Boundary Conditions: Dust Equations

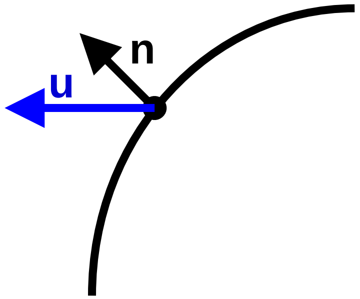
Dirichlet inlet boundary condtions: $u \cdot n < 0$

- Prescribe all conservative variables



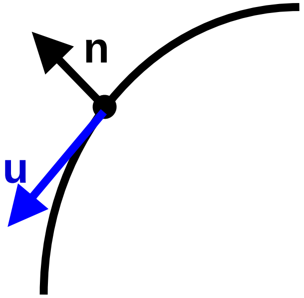
Outlet boundary condtions: $u \cdot n > 0$

- Do nothing



Solid wall condtions: $u \cdot n = 0$

- Project the residual of the momentum equations on the tangent

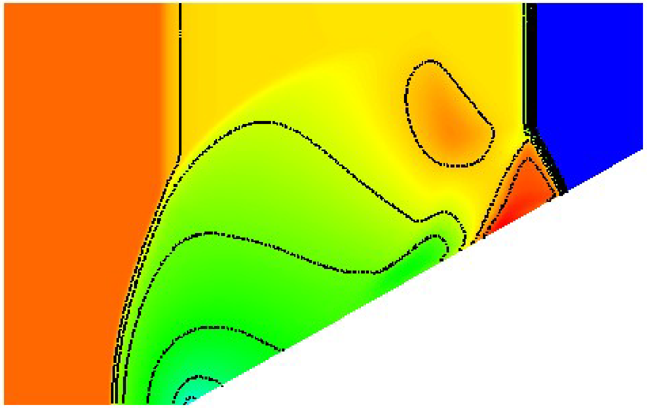


Benchmarking: 2-Fluid Model

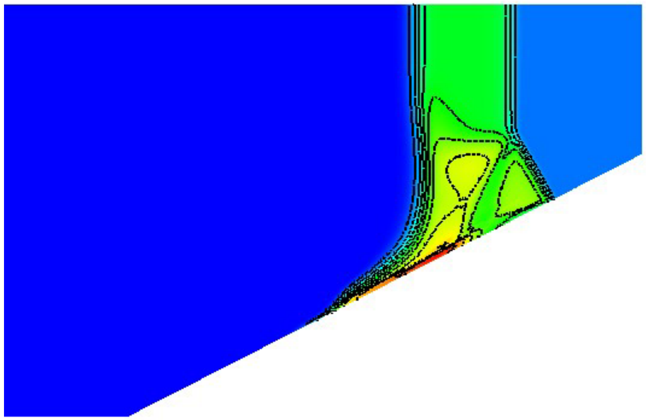
Shock reflection at a compression corner

- Particles are located at the ramp
- Reflection of a shock impinging on the ramp
- Initial velocities at the ramp are zero
- Gas and particles are initially in thermal equilibrium
- Snapshots at time T=0.0007 sec

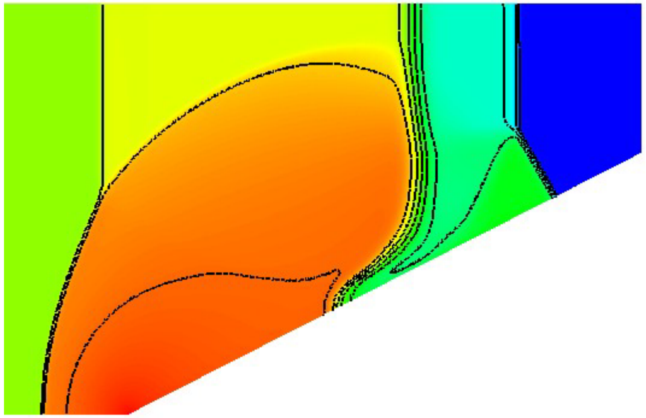
Particle X-velocity



Effective particle density



Particle temperature



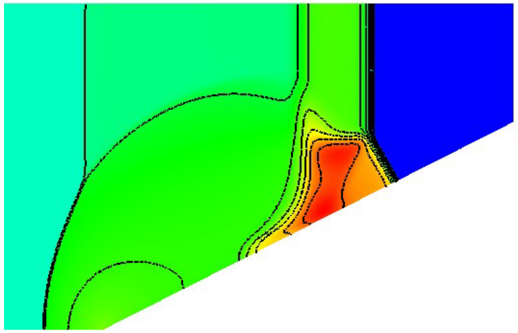
Benchmarking: 2-Fluid Model

Comparison of the gas properties for pure gas and particle-laden gas

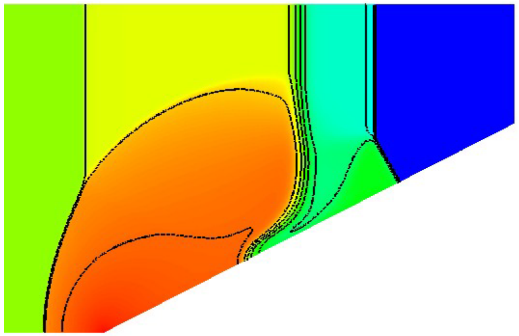
- Snapshots at time T=0.0006 sec

Particle-laden gas

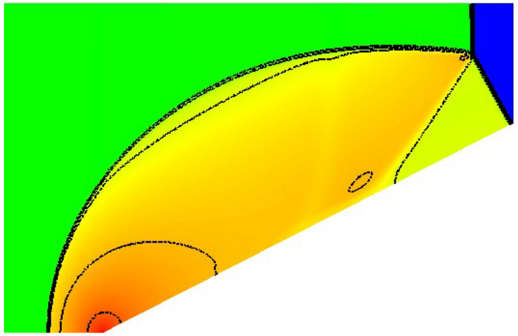
Density

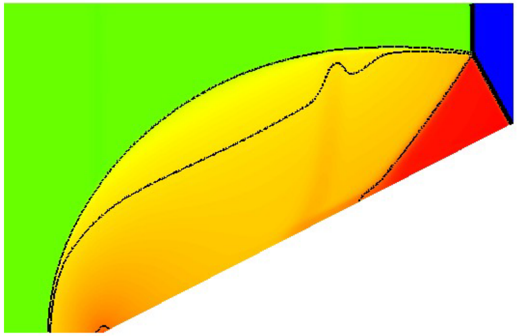


Temperature



Pure gas





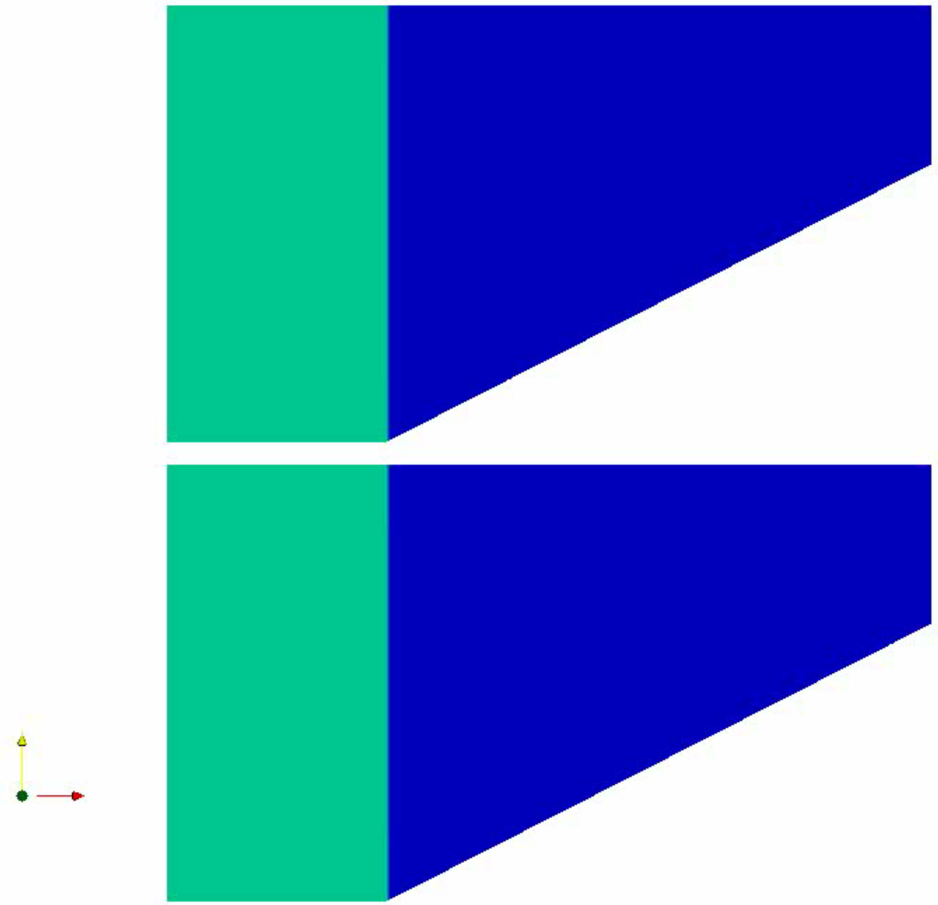
Benchmarking: 2-Fluid Model

Comparison of the gas density for pure gas and particle-laden gas

- Propagation of the shock wave

Particle-laden gas

Pure gas



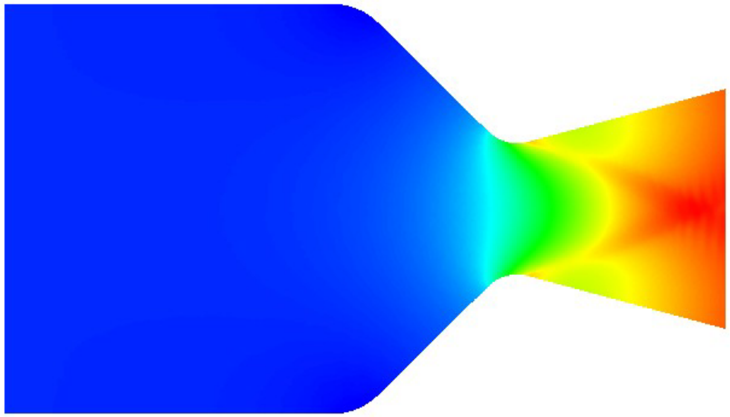
Benchmarking: 2-Fluid Model

Particle-laden nozzle flow

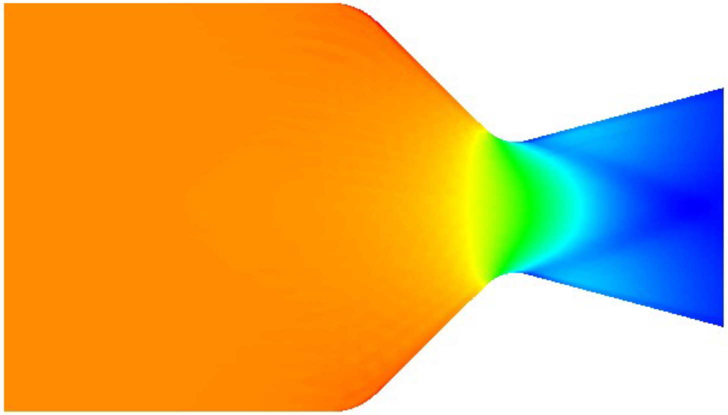
- Curved boundaries
- Wide range of Mach numbers
- Subsonic inlet
- Compressible and incompressible areas
- High stiffness
- Stationary computation

➡ Challenging problem

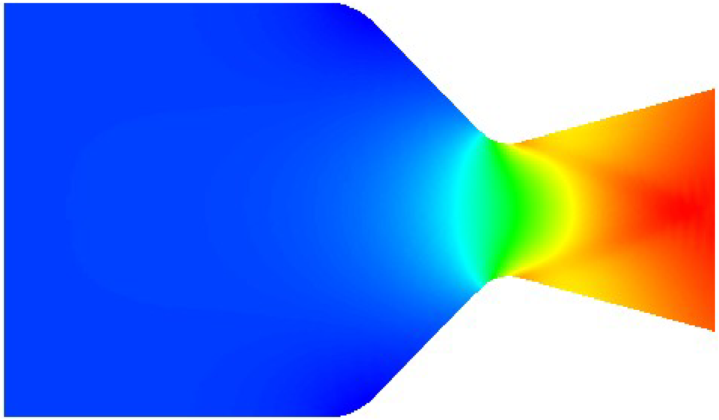
Mach number



Effective particle density



Effective gas density



Conclusions & Outlook

- High resolution TVD-scheme is implemented and validated for several benchmarks
- All the necessary information is inferred from the discrete Galerkin operators
- No restriction to 2D, a generalization to 3D is straightforward
- Further work will focus on the efficiency of steady-state computations
- The FCT approach will be implemented for non-stationary flows
- Adaptivity will be used to reduce the computational cost (Matthias Möller)