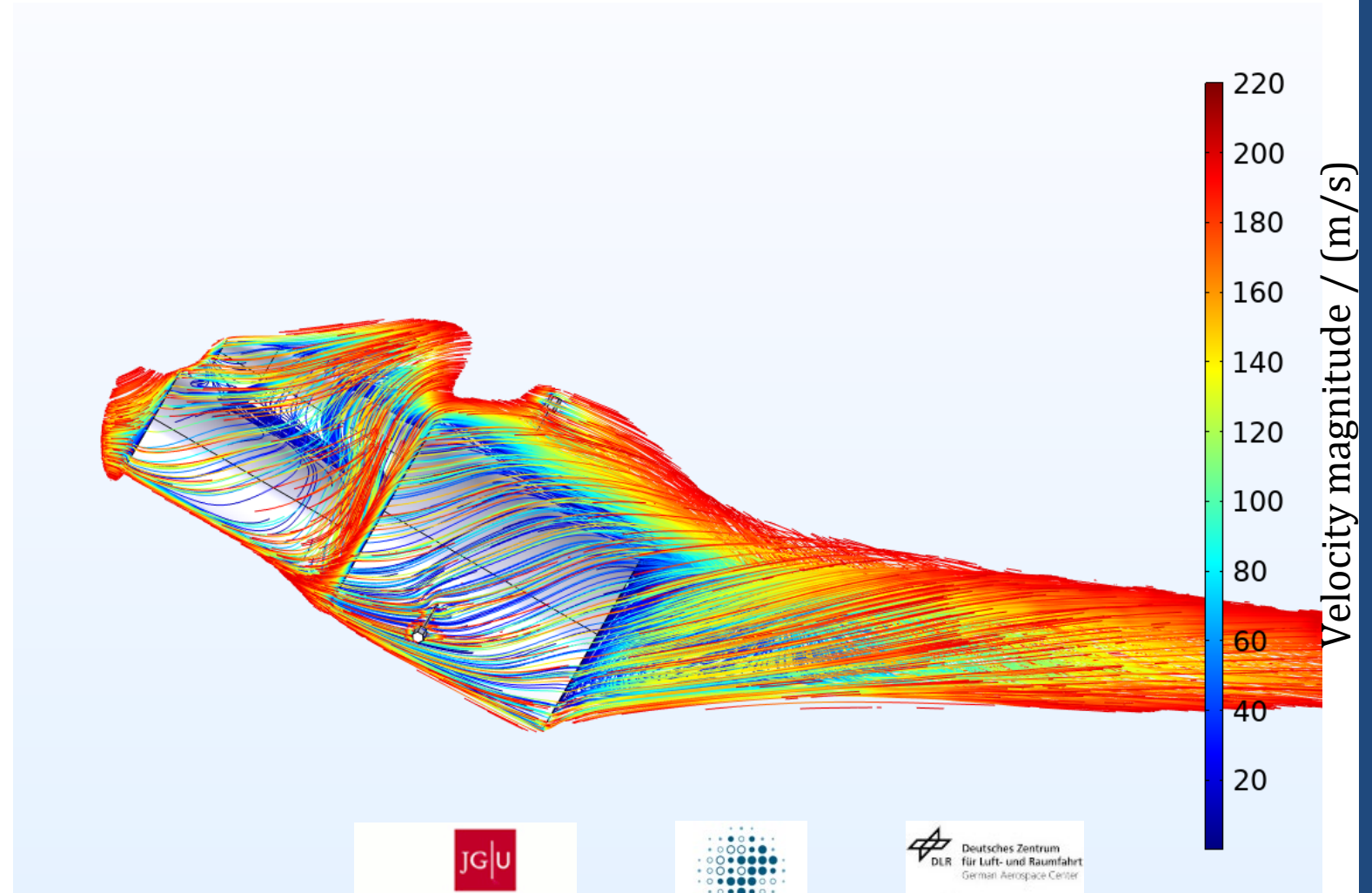


COMSOL simulations to develop and investigate the efficiency of a rocket-borne particle collector

Birte Klug

COMSOL
MULTIPHYSICS®





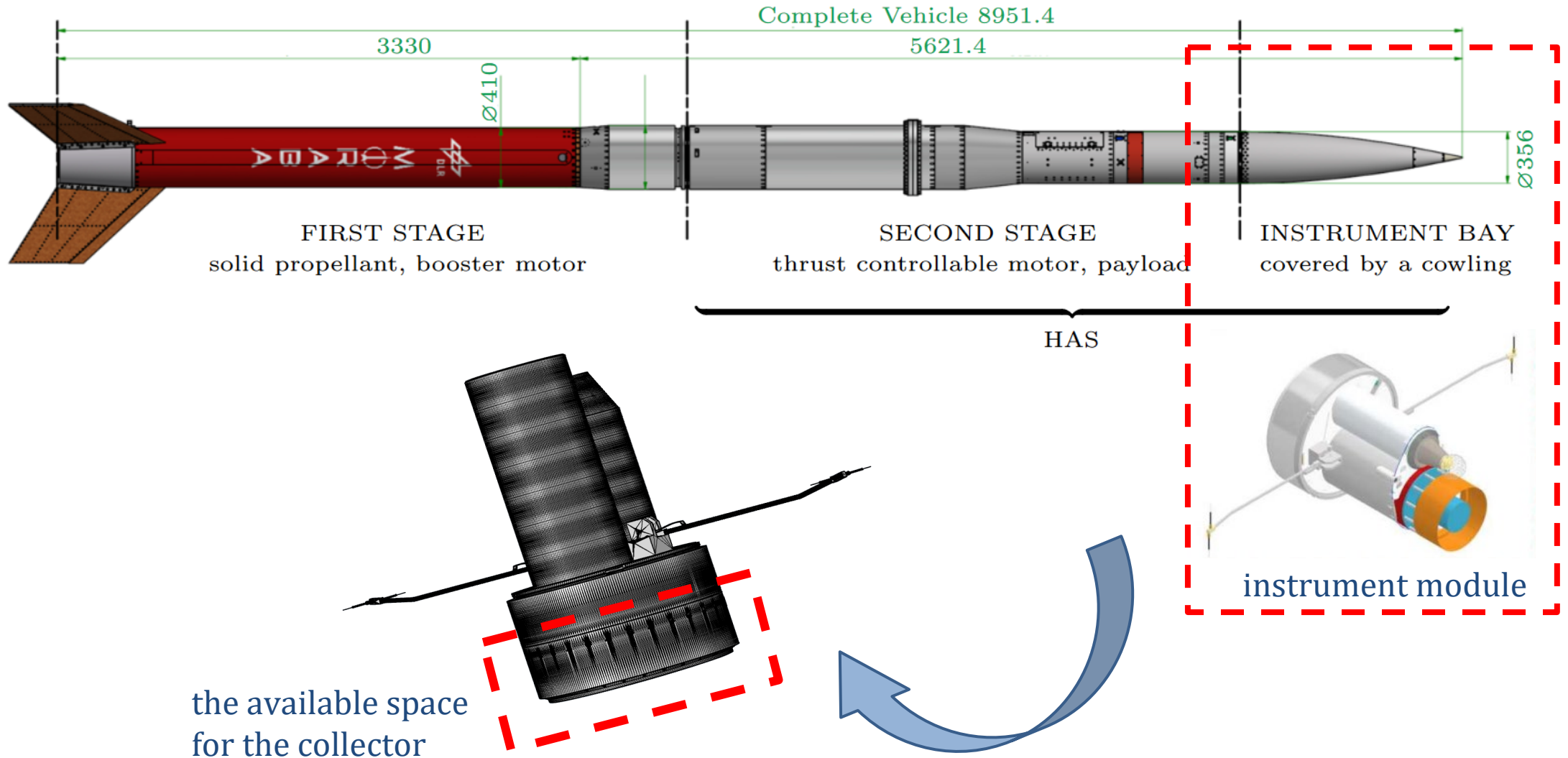
Altitude:
~85 km

Idea:

Sampling based, free-stream impactor

- Collection of particles on the surface of a flow obstacle
- Analysis of the particles

Rocket



Mathematical and numerical
model of supersonic flows
around the instrument module

Supersonic flow regime

rocket speed

$$v = 300 - 400 \frac{\text{m}}{\text{s}}$$

speed of sound

$$c_{85 \text{ km}} \approx 230 \frac{\text{m}}{\text{s}}$$

Mach number

$$Ma = 1.3 - 1.8$$

High Mach Number Flow, Laminar (hmnf) interface ()

Compressible Navier Stokes equations

continuity equation

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

momentum equation

$$\frac{\partial(\rho\vec{u})}{\partial t} + \nabla \cdot (\rho\vec{u}\vec{u}^T) = \nabla \cdot \mathbf{T}_f + \rho\vec{f}$$

energy equation

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\rho\vec{u}E) = -\nabla \cdot k\nabla T + Q + \nabla \cdot (\mathbf{T}_f\vec{u}) + \rho(\vec{f} \cdot \vec{u})$$

internal energy equation
ideal gas law

$$\text{with } E = e + \frac{u^2}{2}, \text{ and } e = c_v T, \rho = \frac{p}{R_s T},$$

$$\mathbf{T}_f = -p\mathbf{I} + \left[\mu \left(\nabla\vec{u} + (\nabla\vec{u})^T - \frac{2}{3}(\nabla \cdot \vec{u})\mathbf{I} \right) \right]$$

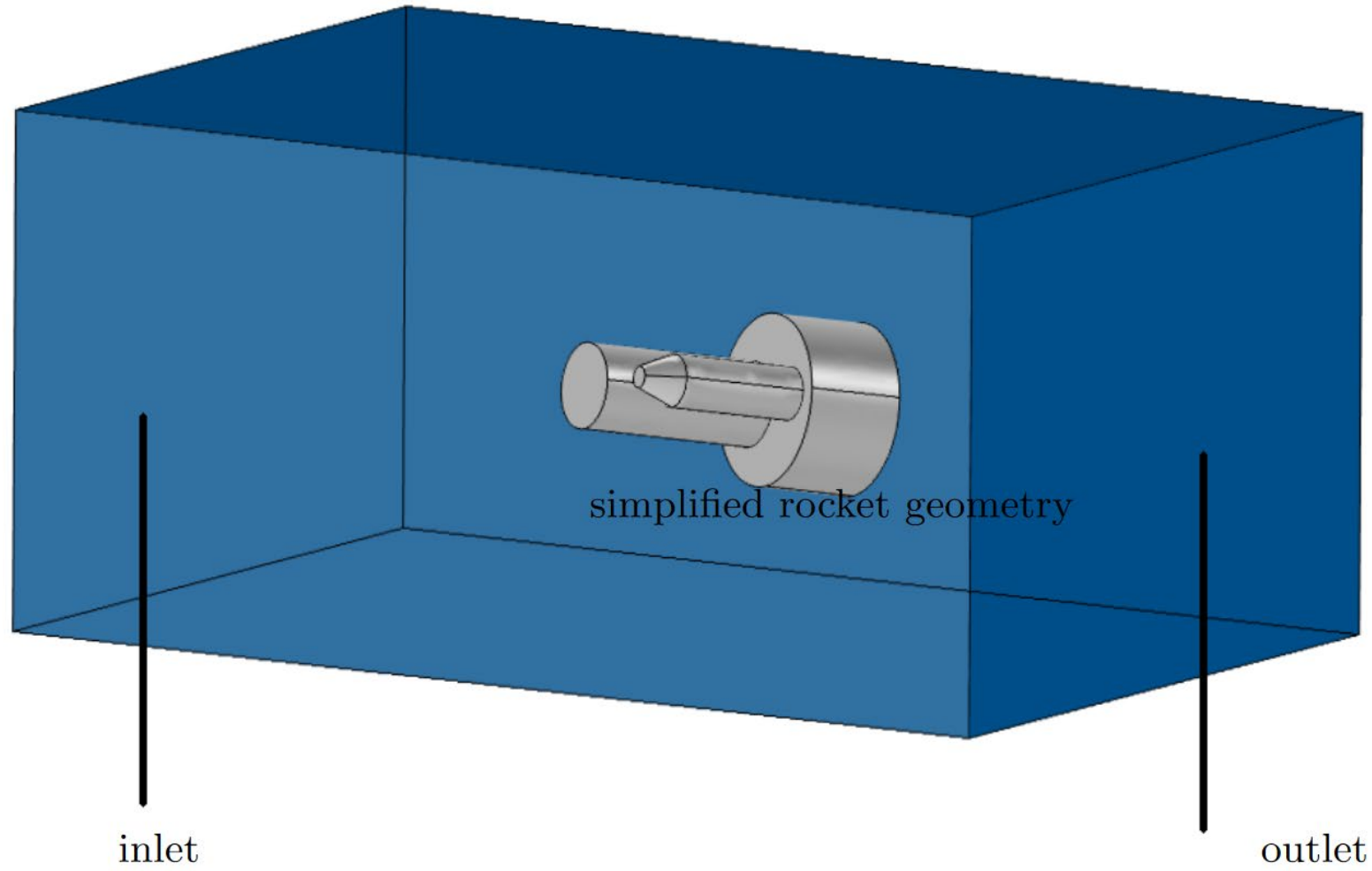
ρ : density
 \vec{u} : velocity
 p : pressure

μ : dynamic viscosity
 \vec{f} : body force
 e : internal energy

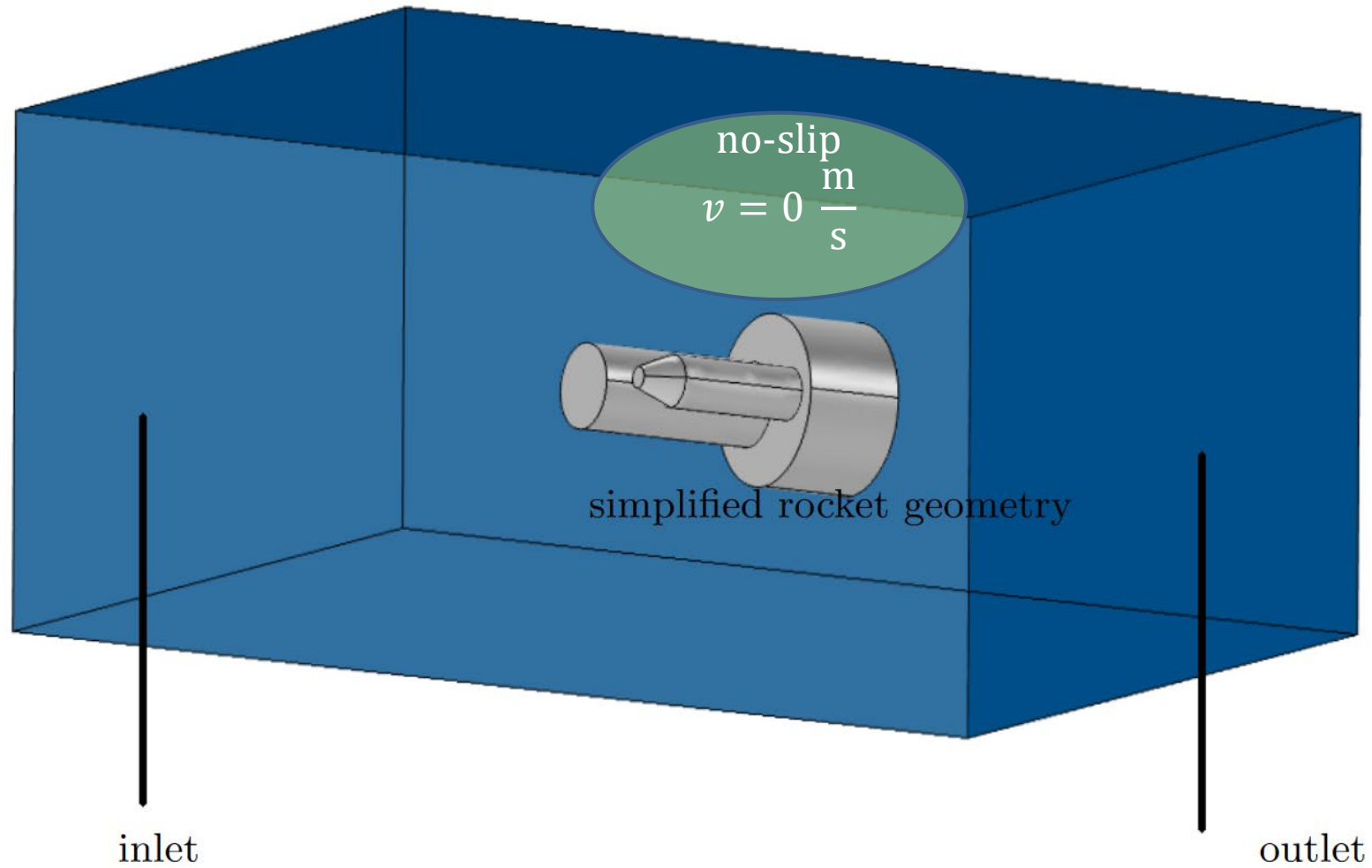
c_v : specific heat capacity
 T : temperature
 R_s : specific gas constant

$\vec{q} = k\nabla T$: heat flow vector
 k : thermal conductivity

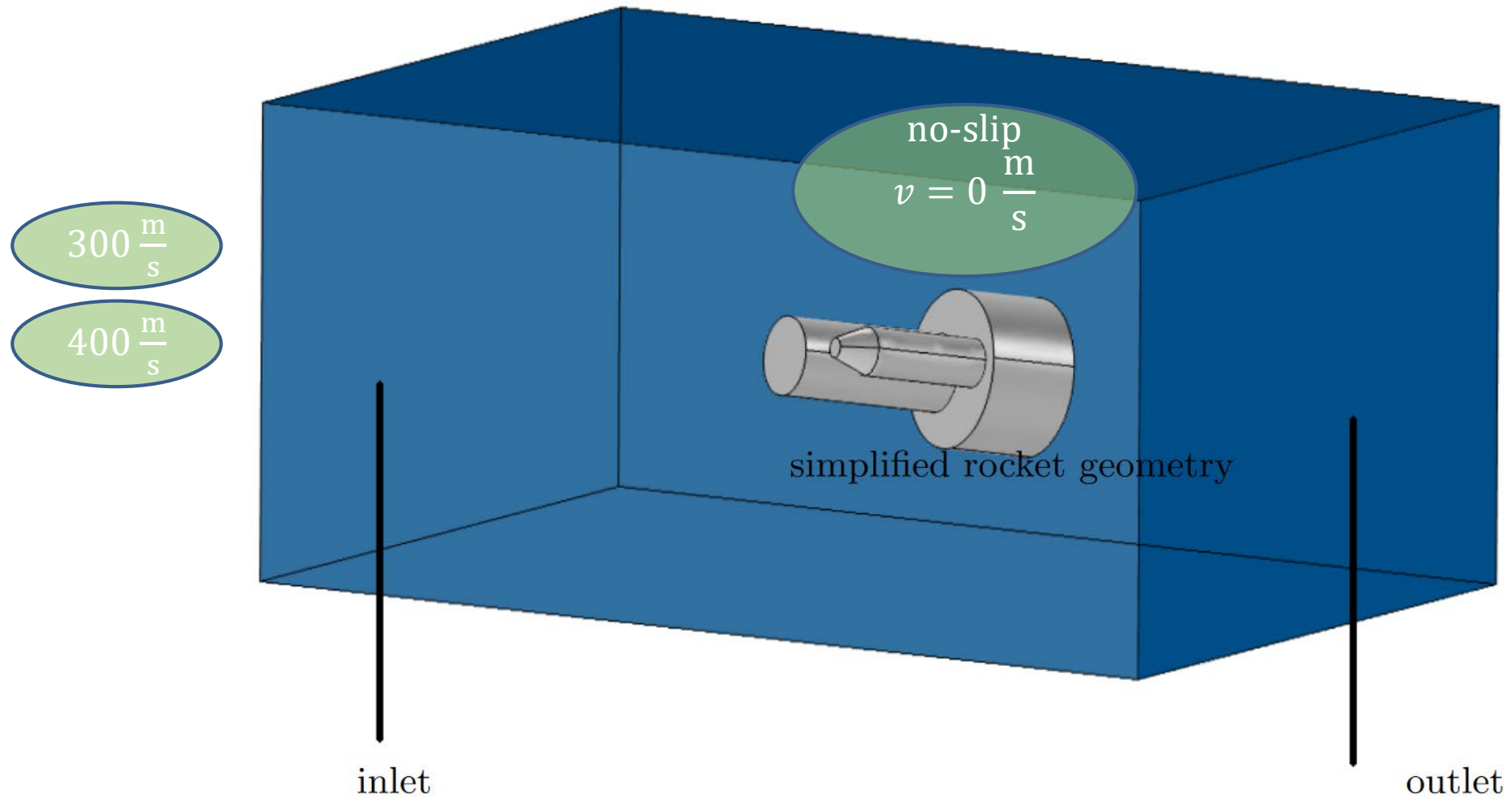
Simulation geometry



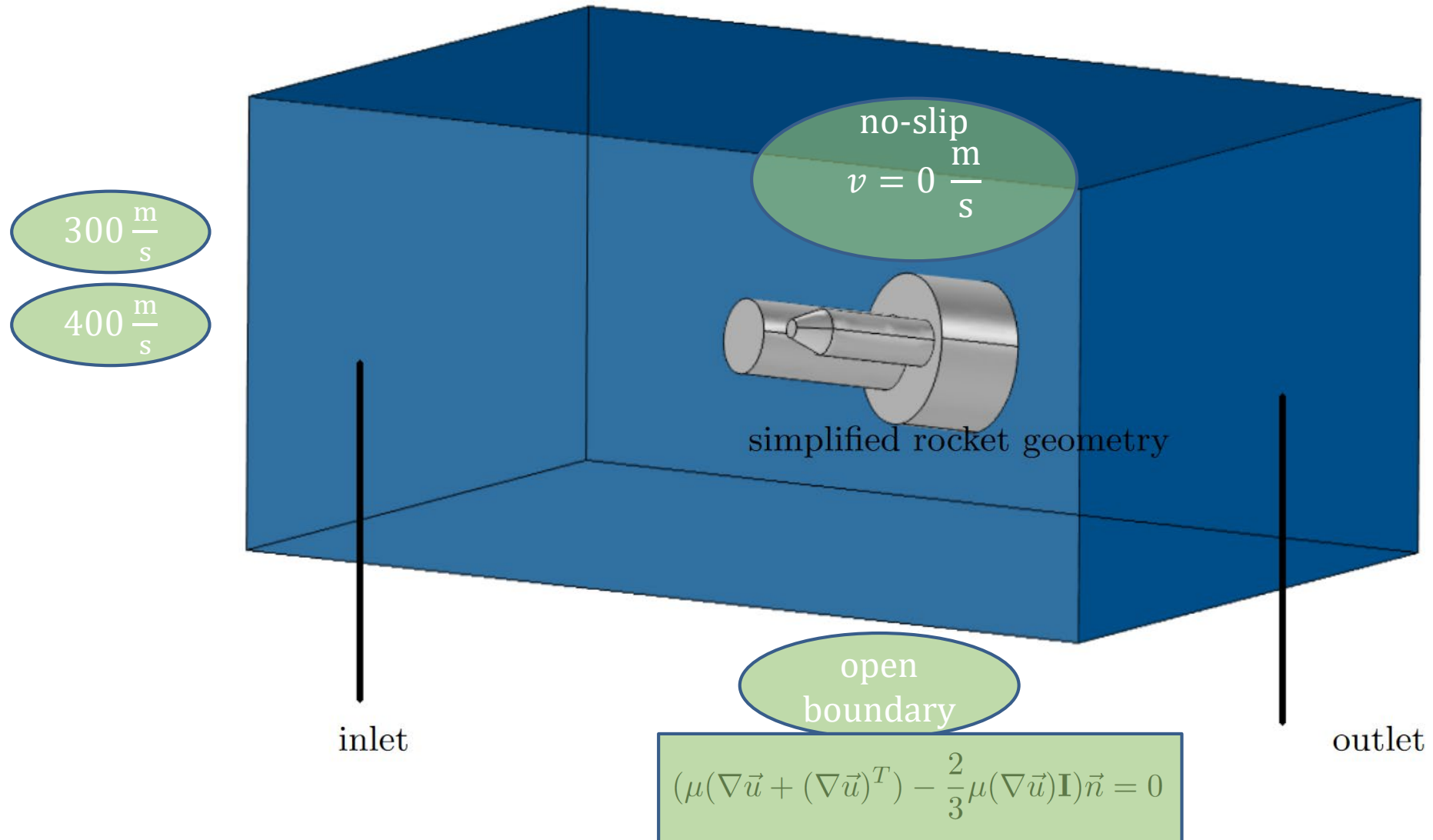
Simulation geometry



Simulation geometry



Simulation geometry

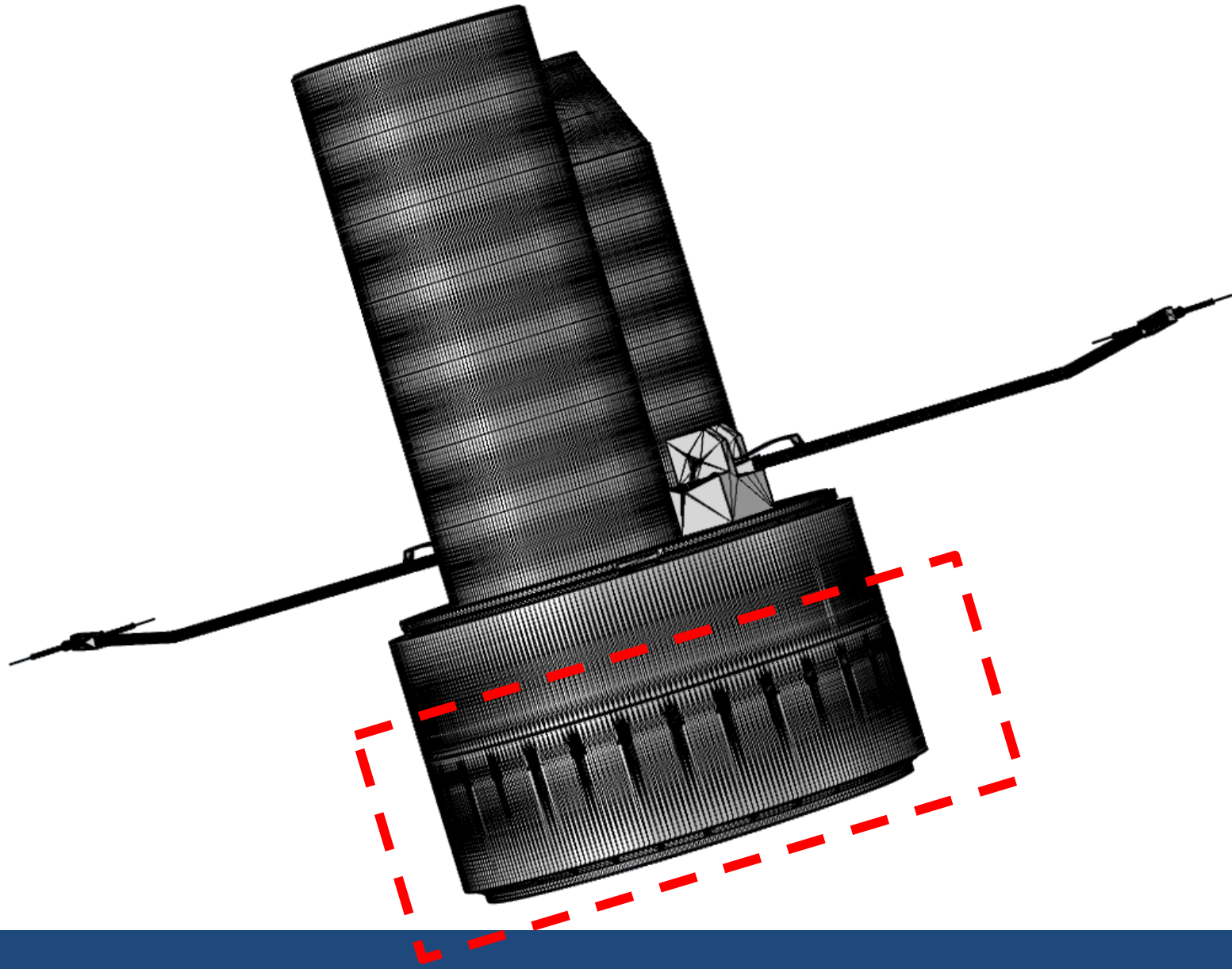


Computing data of our COMSOL model

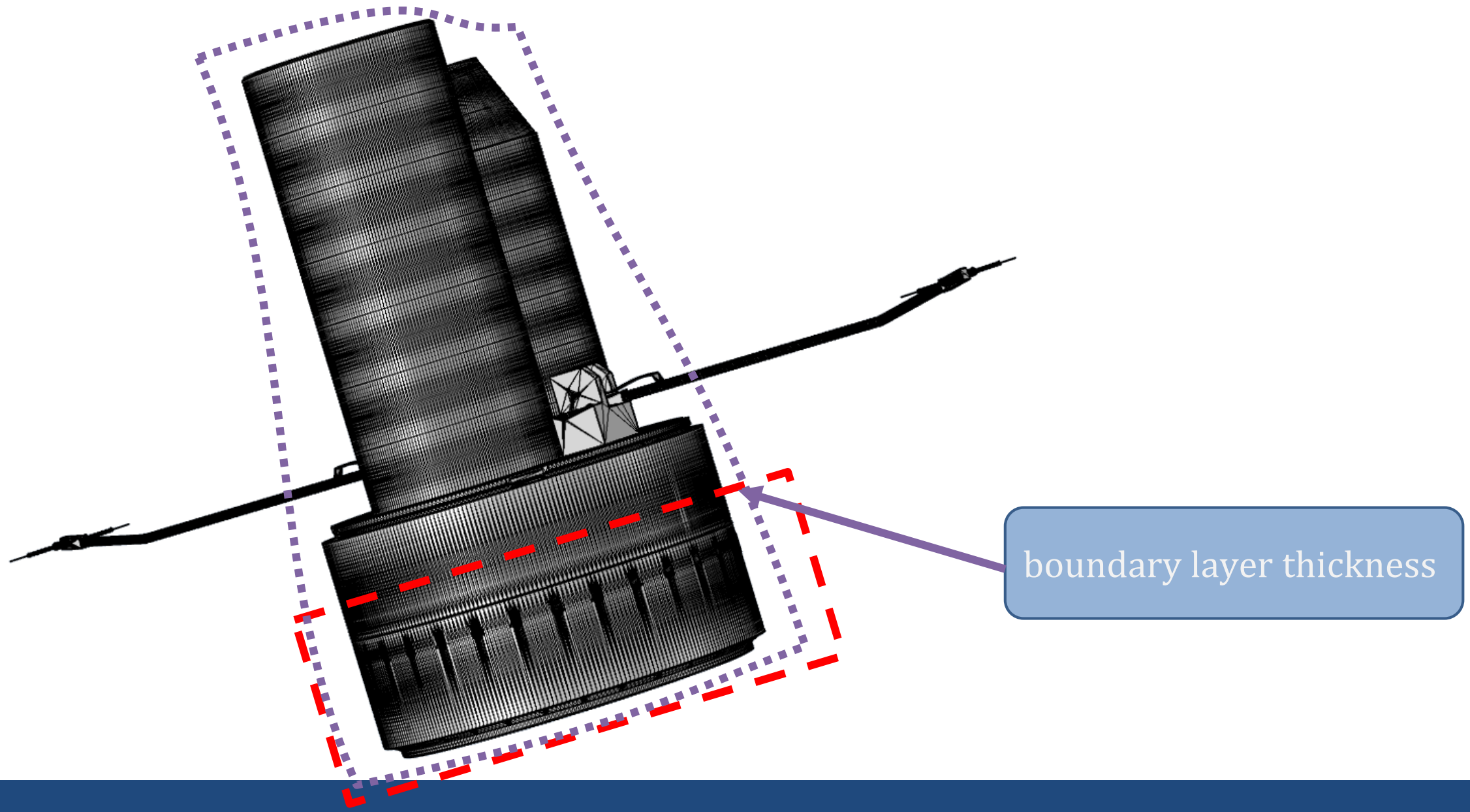
- Combination of tetrahedral, pyramidal, prismatic mesh elements
- ~4 million mesh elements
- Smallest element sizes: ~ 1 mm
- Time discretization by BDF (backward differentiation formula) method
- Cluster computing:
 - 6 nodes
 - 70 cores
 - 396 GB RAM (working storage)
- Solving time up to 20 days

Simulation based development of the particle collector

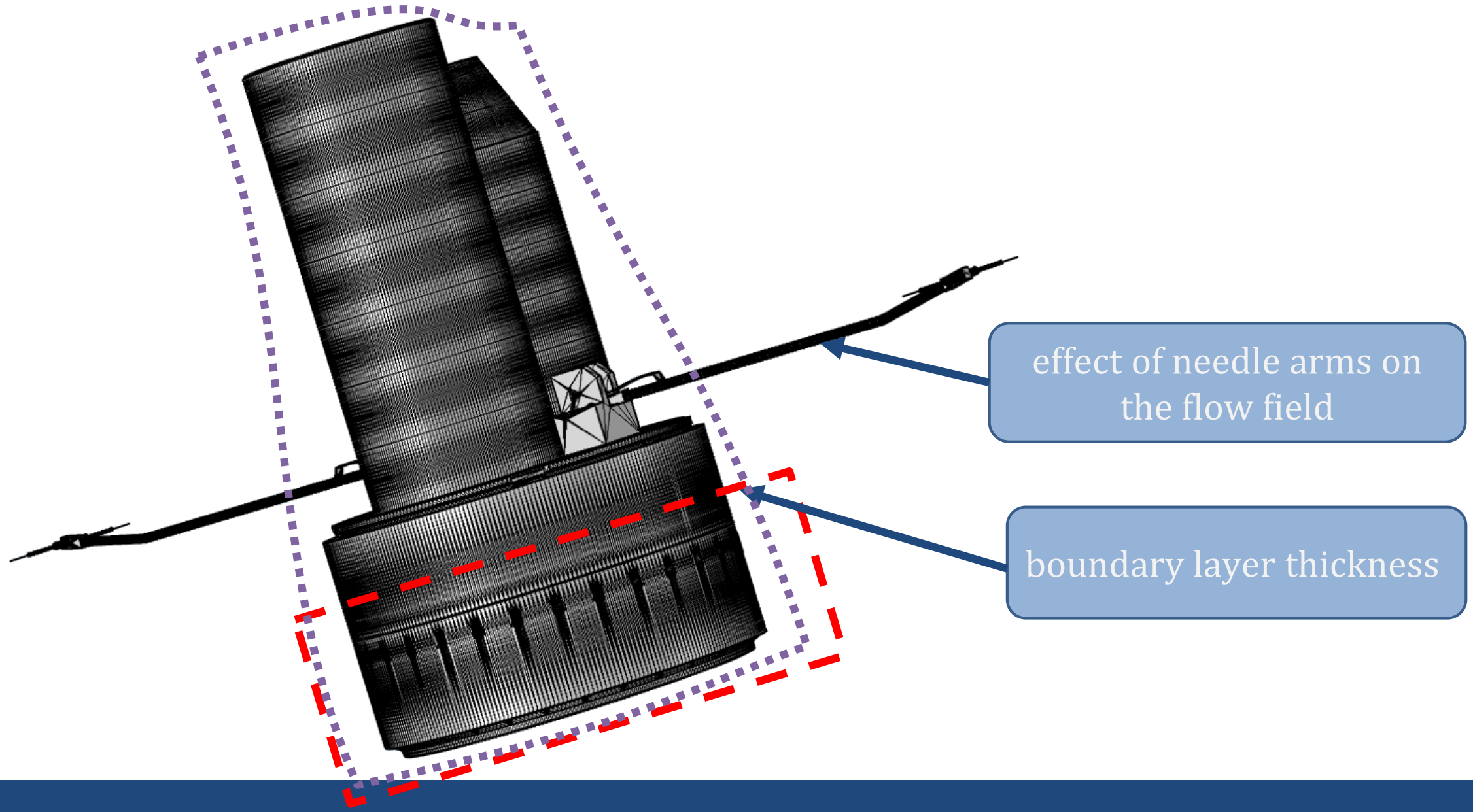
Development of the particle collector



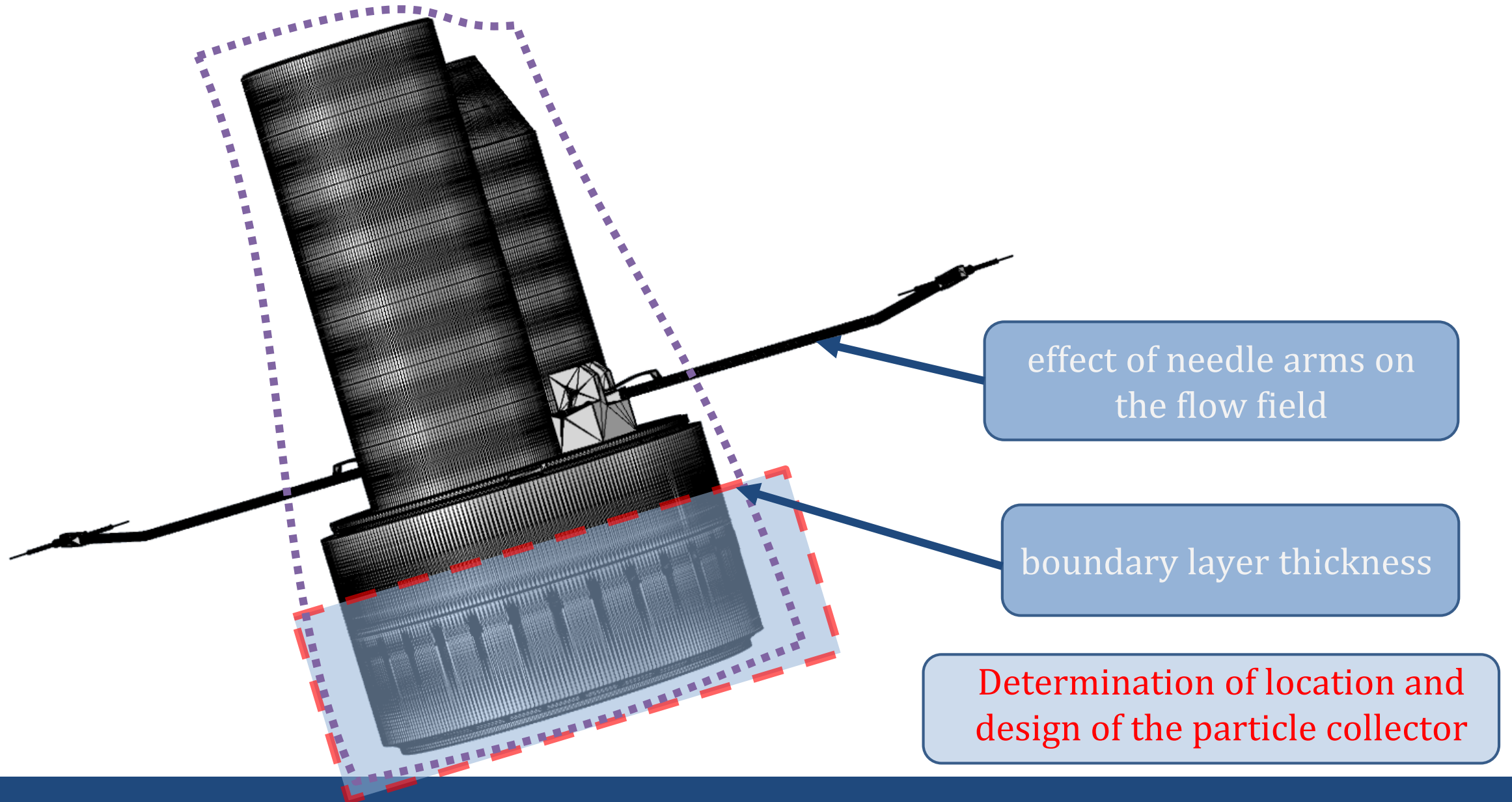
Development of the particle collector



Development of the particle collector



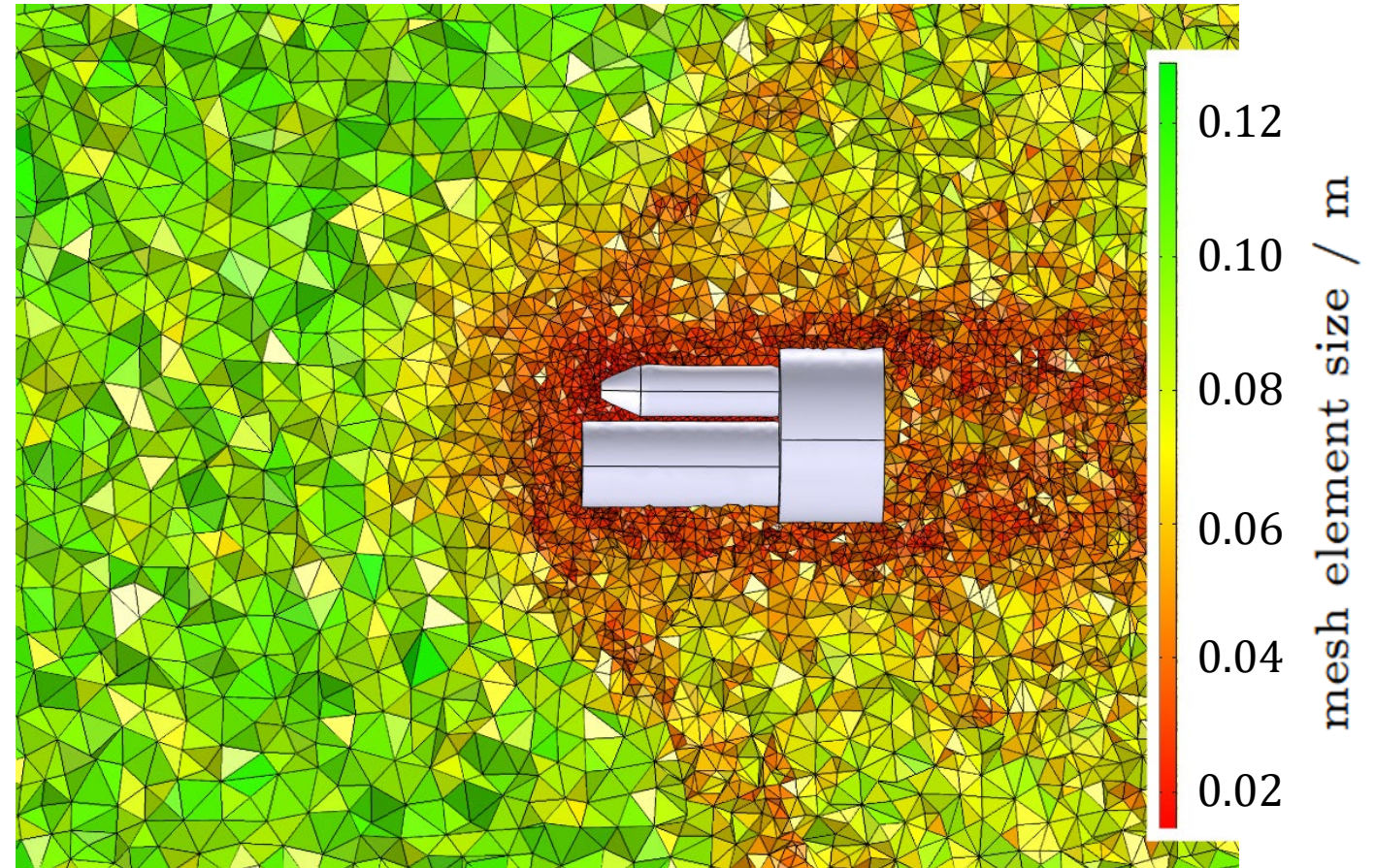
Development of the particle collector



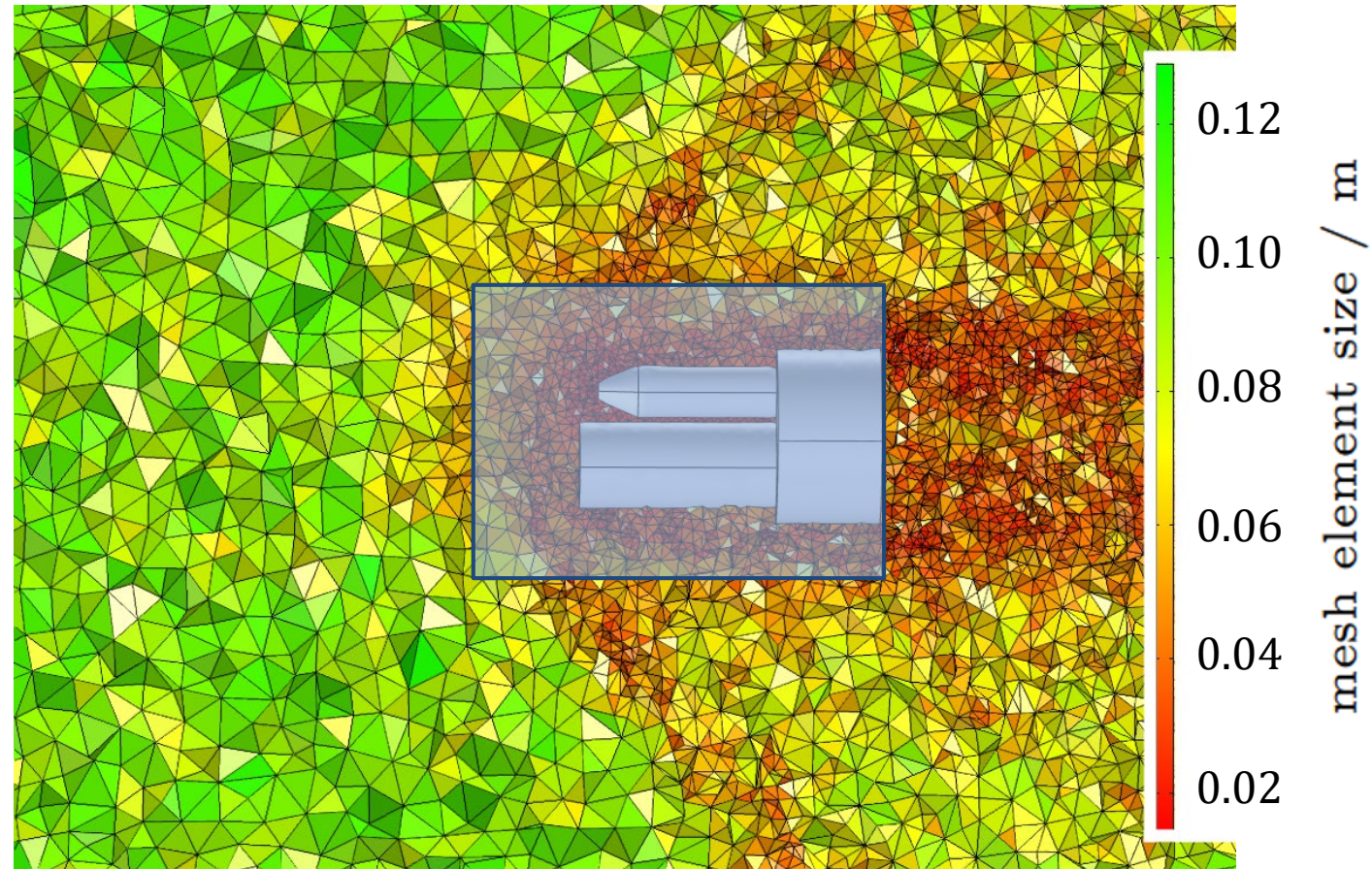
Generated 3D mesh for simulations

Mesh refinement by the
error indicator:

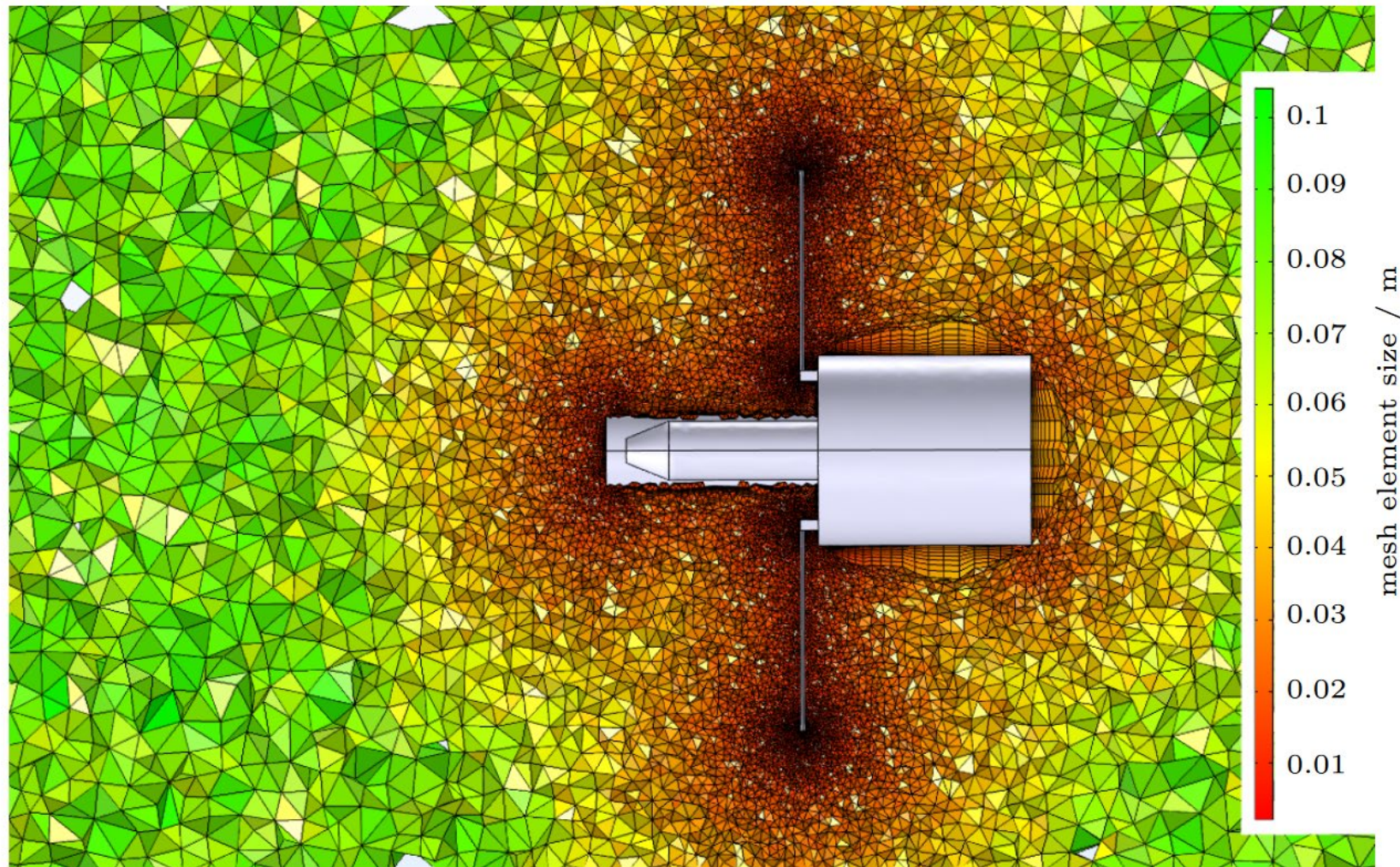
$$\|\nabla \vec{u}\|$$



Generated 3D mesh for simulations

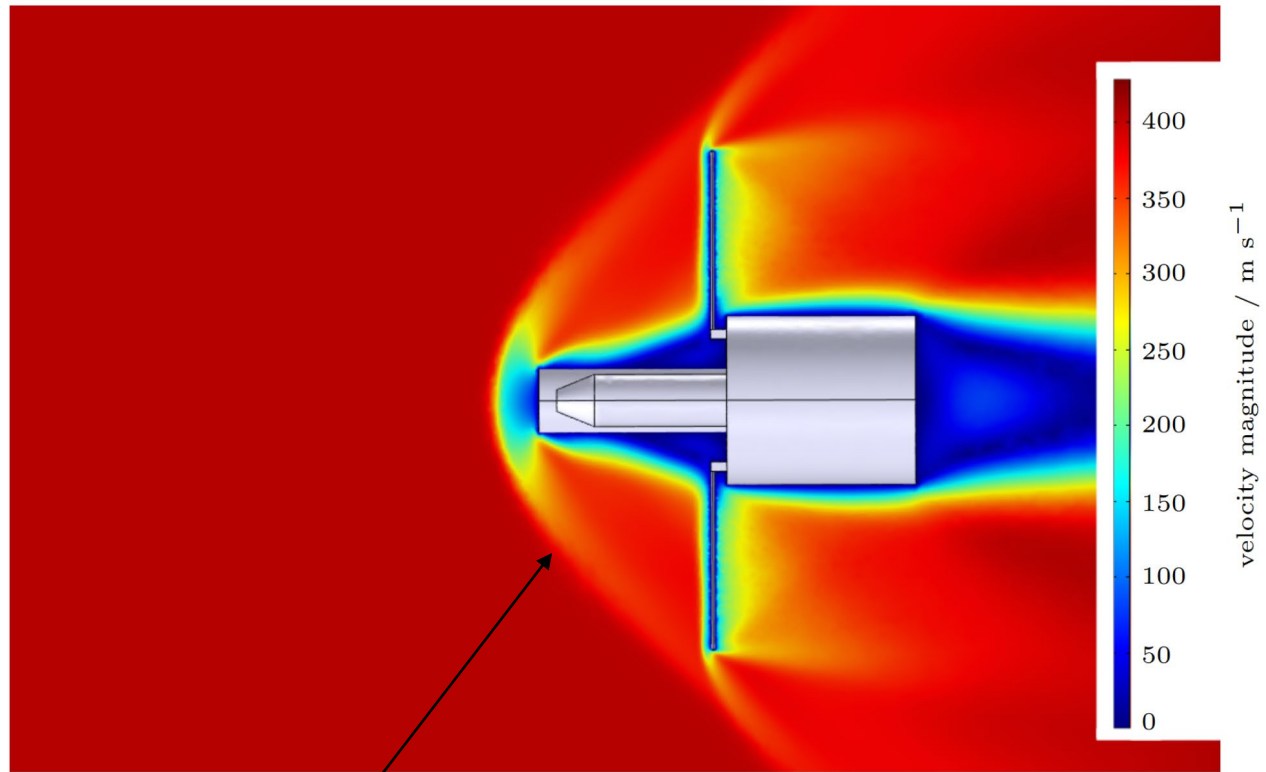


Generated 3D mesh for simulations

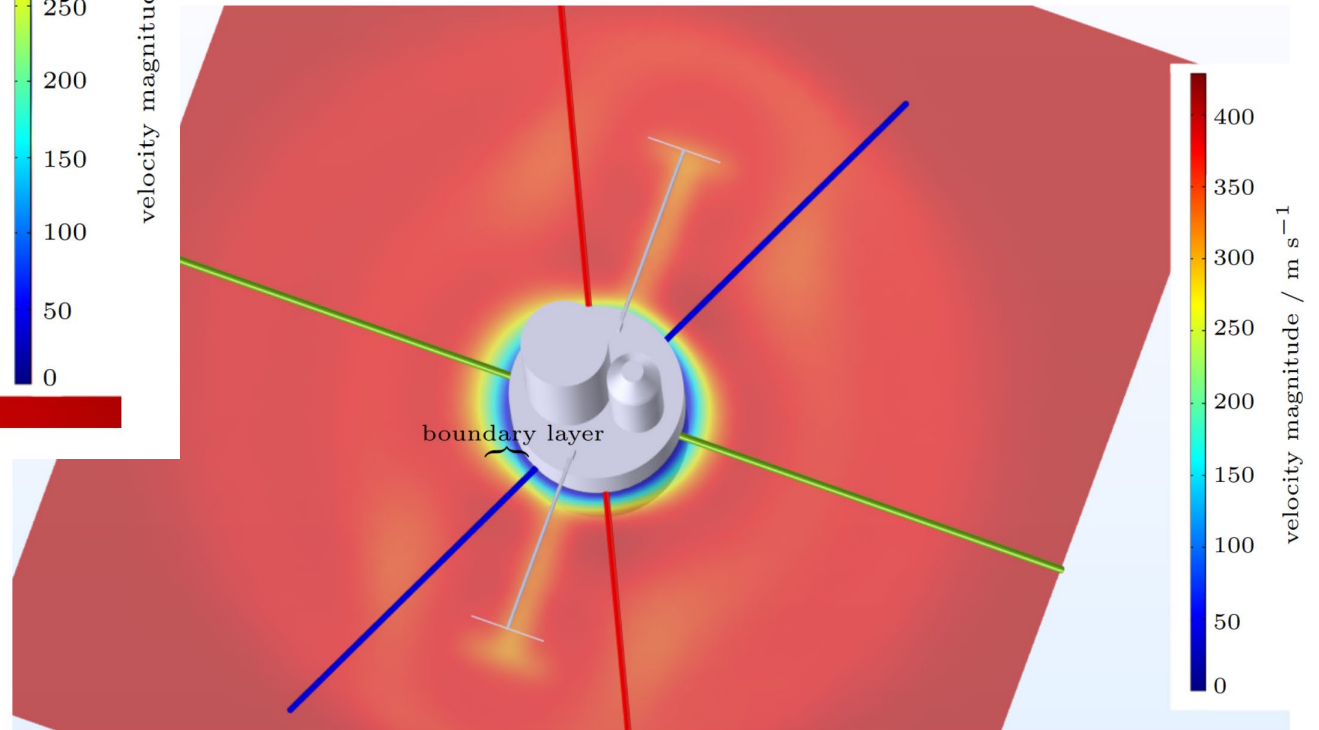


Mesh element size in m

Flow field around the payload tip

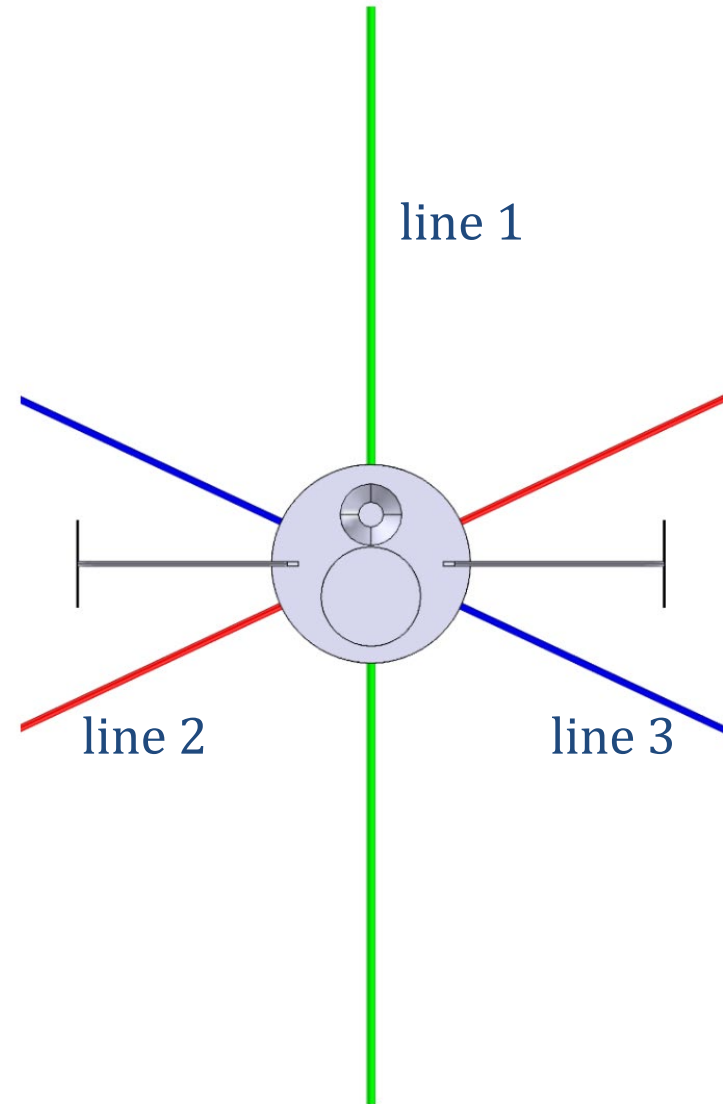
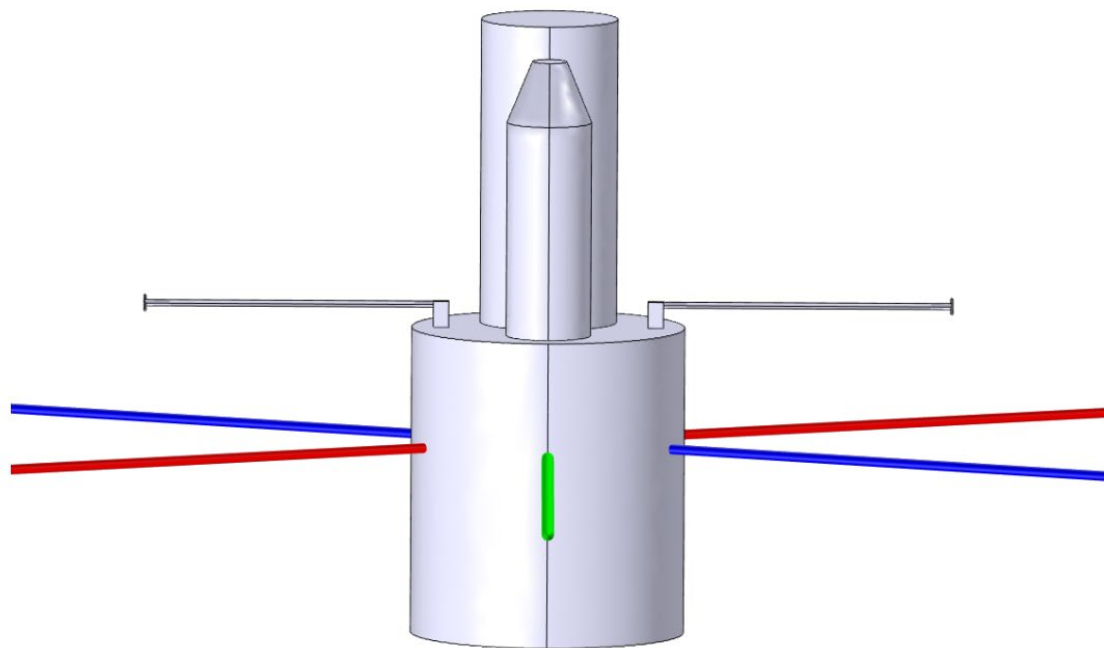


shock wave

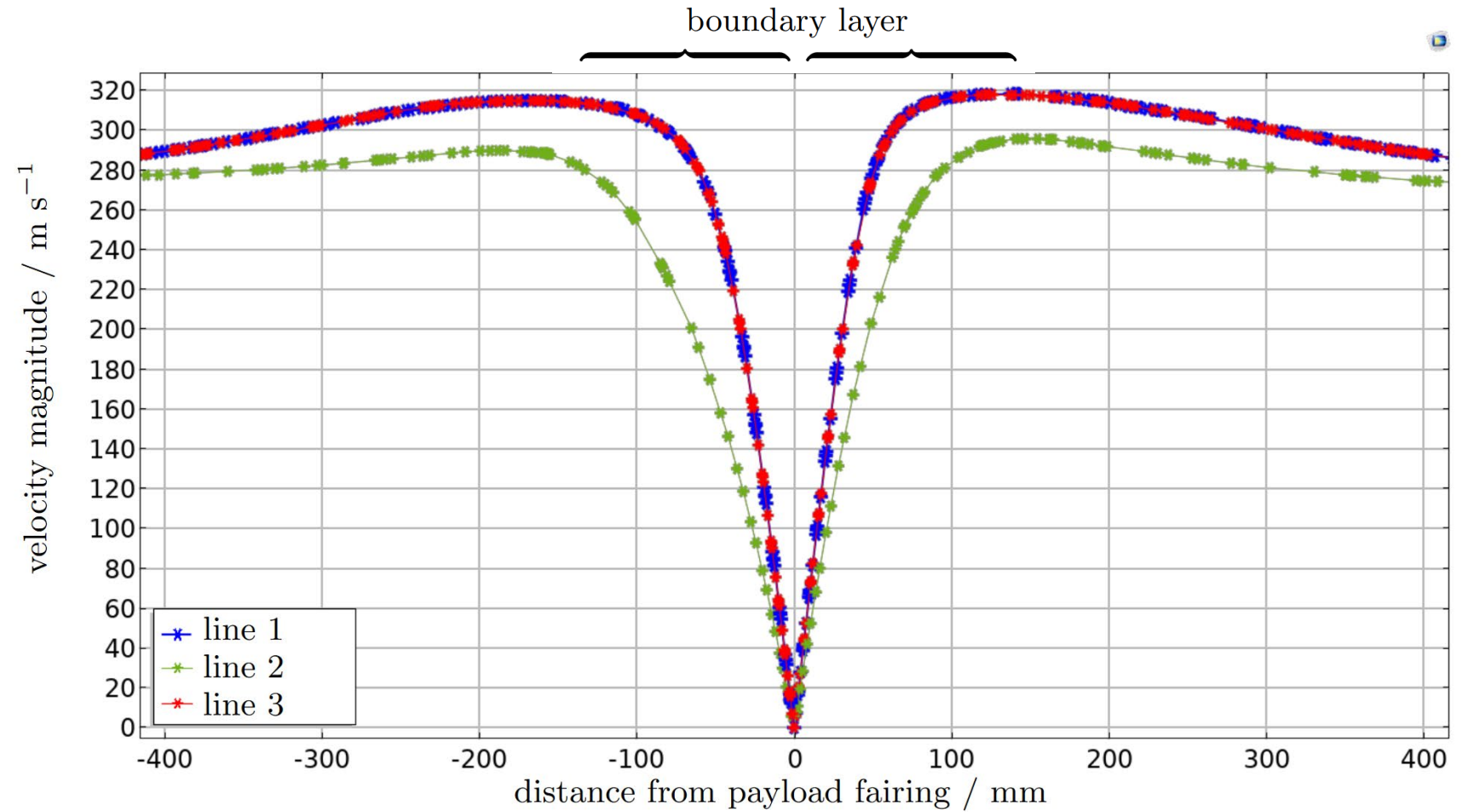
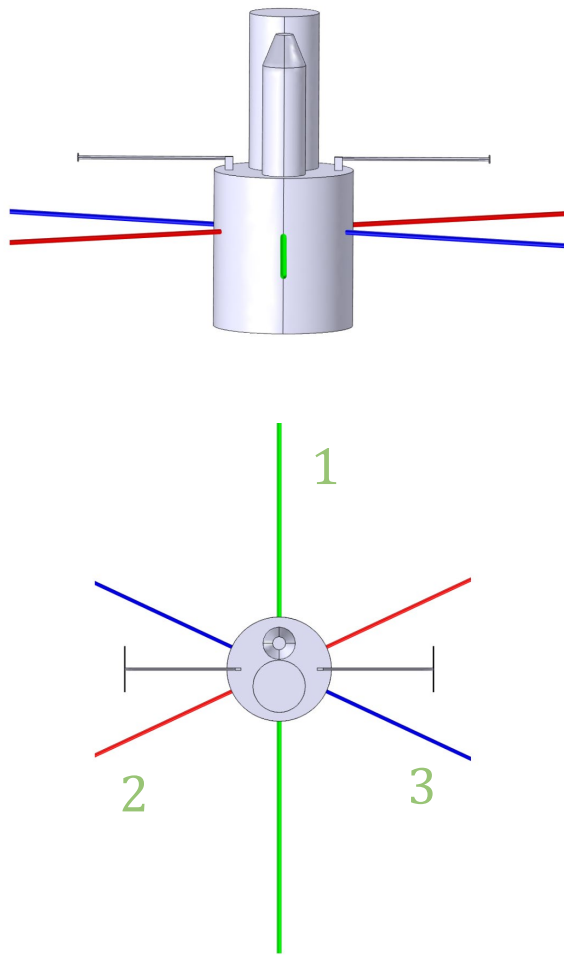


Velocity magnitude depicted on a cut plane perpendicular to the payload tip

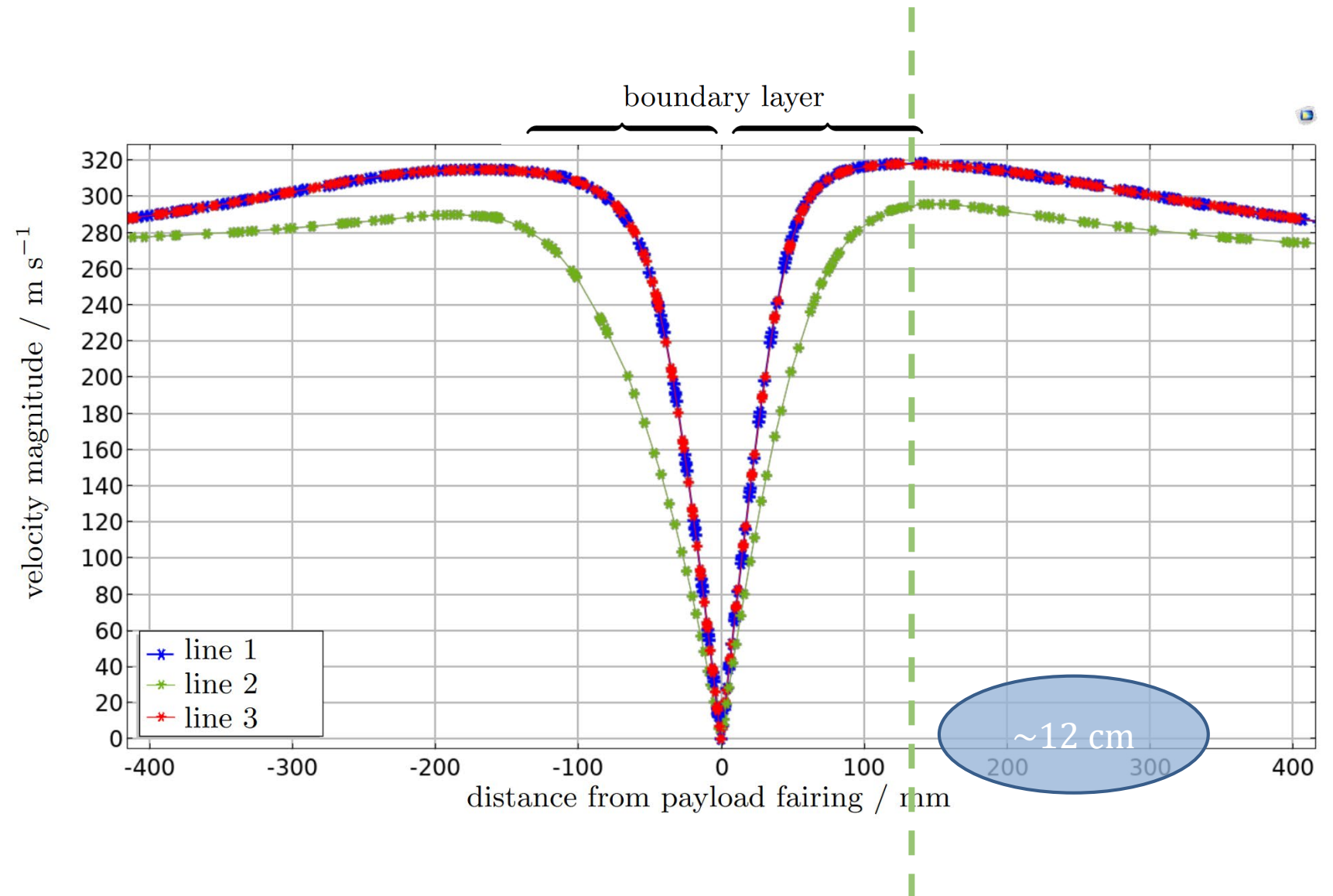
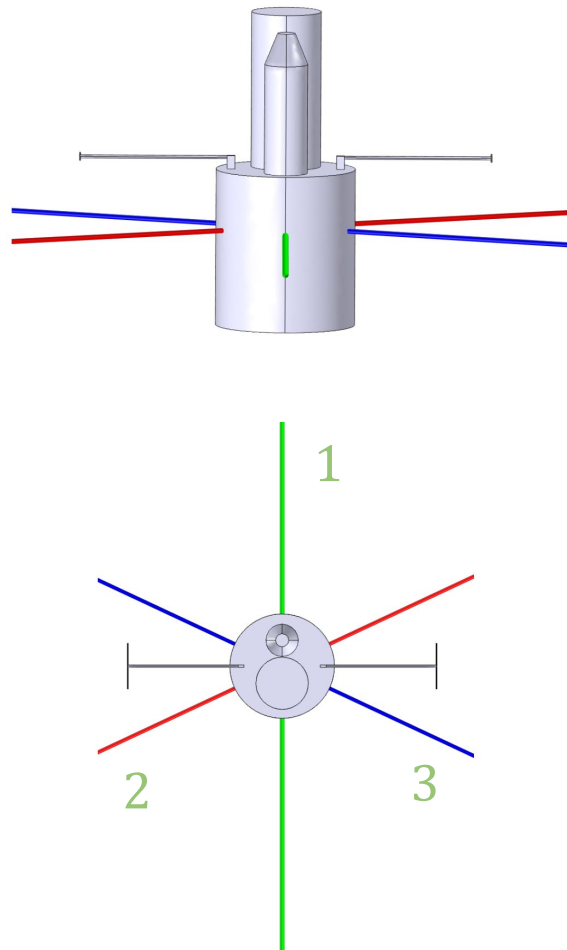
Analyzing velocity magnitudes along cut lines



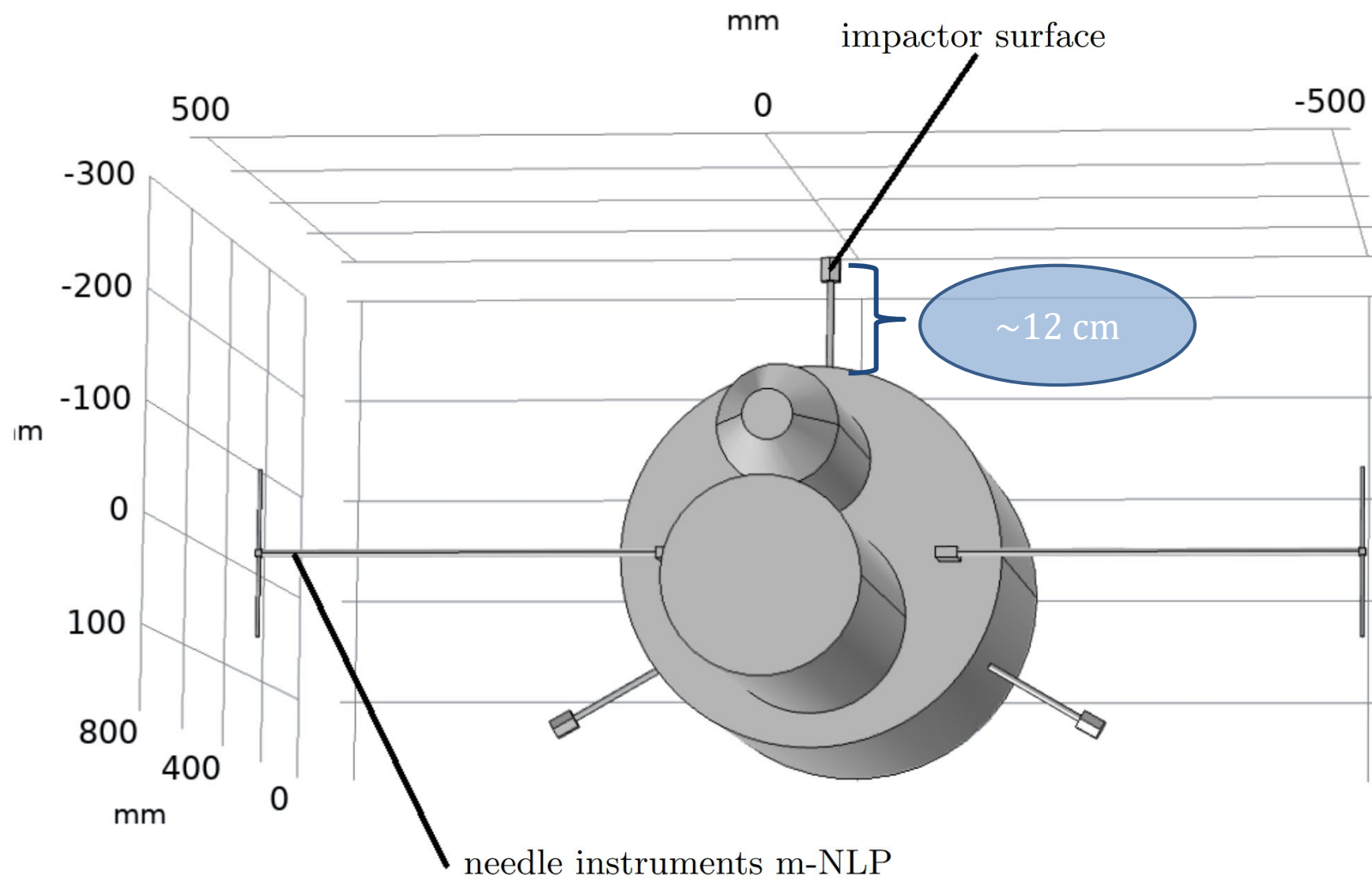
Analyzing velocity magnitudes along cut lines



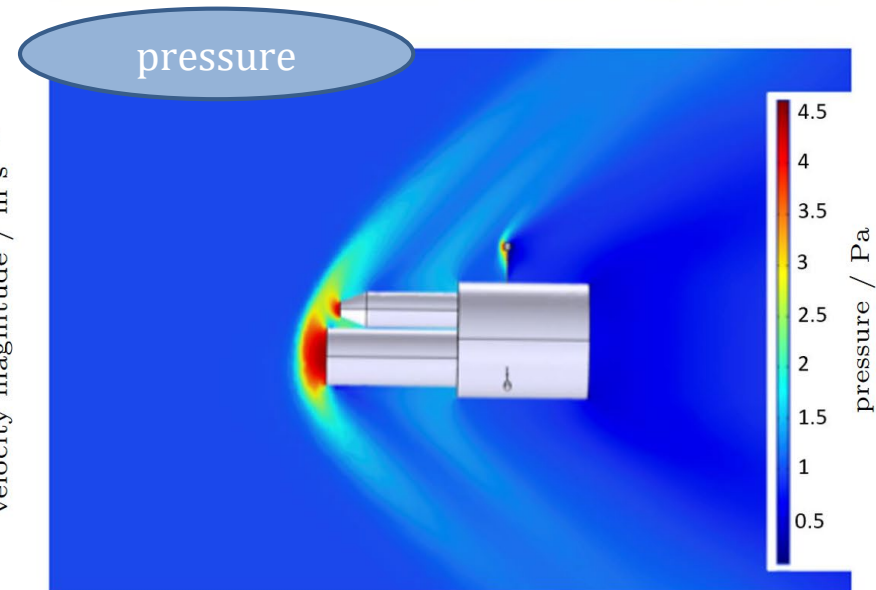
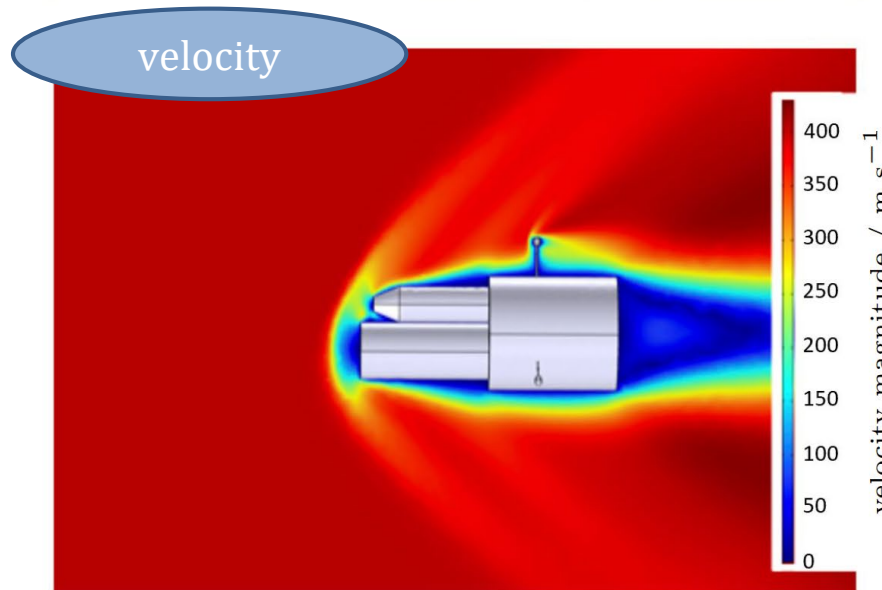
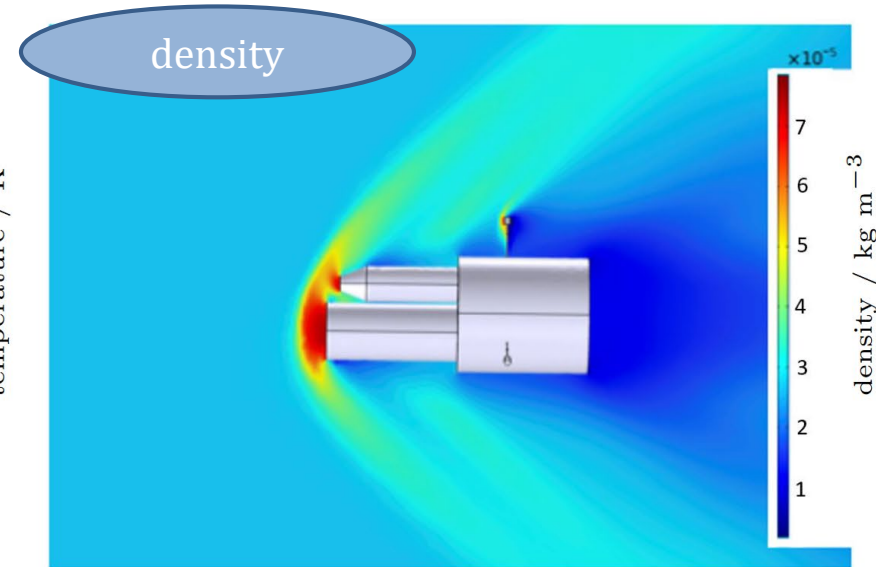
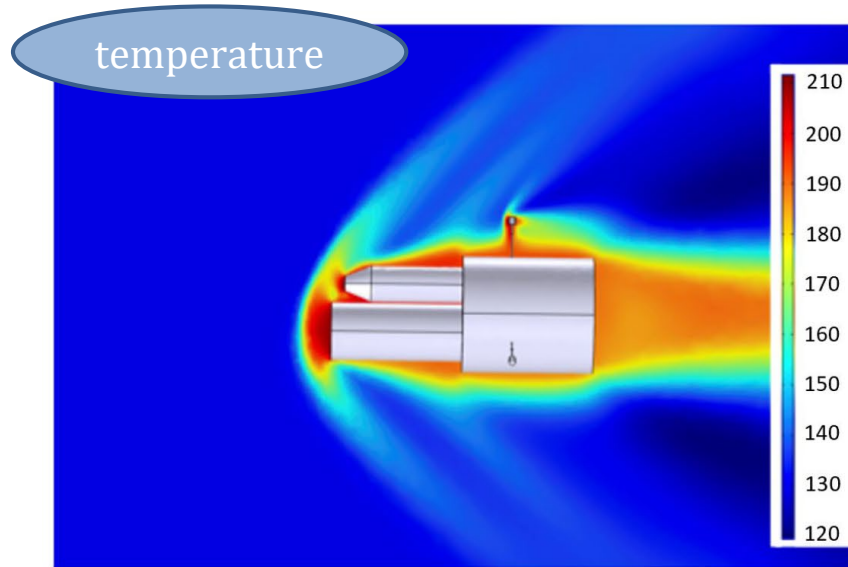
Analyzing velocity magnitudes along cut lines



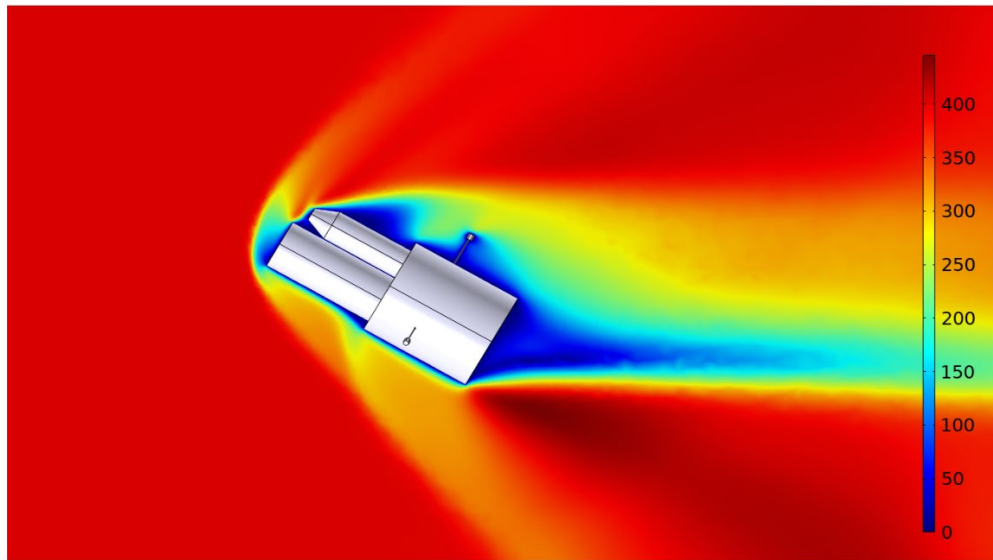
Final location and design of the samplers



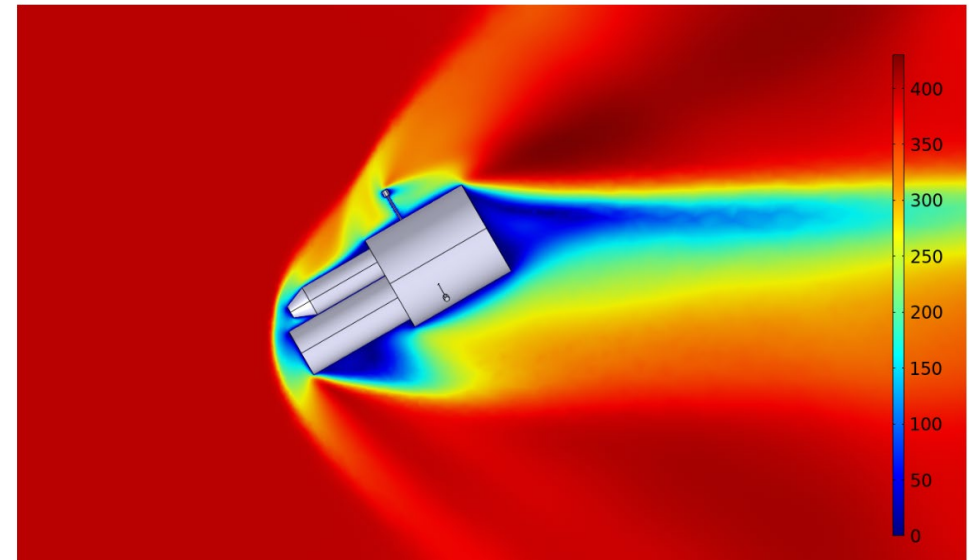
Flow field around the payload tip 0° angle of attack



Flow field around the payload tip at $\pm 30^\circ$ angle of attack



velocity magnitude / m s^{-1}



velocity magnitude / m s^{-1}

Mathematical and numerical model of particle simulations

Particle data

Particle volume fraction

$$\Phi_p = \frac{nV_p}{V} \leq 10^{-6}$$



one-way
coupling

Knudsen number

$$Kn_p = \frac{2\lambda}{d_p} > 1$$

Cunningham
slip corrector

n : number of particles

V_p : particle volume

V : fluid volume

Kn_p : Knudsen number

λ : mean free path

d_p : particle diameter

Estimation of particle forces

| forces | mathematical expressions | estimated magnitude of forces / N |
|-------------------------|---|-----------------------------------|
| Brownian force | $\vec{F}_{Brown} = \zeta \sqrt{\frac{6 \pi \mu k_B T d_p}{\Delta t C_c}}$ | $\sim 10^{-18}$ |
| Stokes drag force | $\vec{F}_D = 3 \pi \mu_f d_p \vec{u}_r C_c^{-1}$ | $\sim 10^{-18}$ |
| Saffman force | $\vec{F}_S = 1.615 d_p^2 \vec{L}_f \sqrt{\rho_f \mu_f \frac{1}{ \nabla \times \vec{u}_r }}$ | $\sim 10^{-22}$ |
| gravitational force | $\vec{F}_{G,tot} = m_p \frac{\rho_p - \rho_f}{\rho_p} \vec{g}$ | $\sim 10^{-23}$ |
| added mass force | $\vec{F}_{am} = m_f c_{am} \frac{d(\vec{u}_f - \vec{v}_p)}{dt}$ | $\sim 10^{-25}$ |
| pressure gradient force | $\vec{F}_p = -\frac{m_p}{\rho_p} \nabla p$ | $\sim 10^{-28}$ |

Estimation of particle forces

| forces | mathematical expressions | estimated magnitude of forces / N |
|-------------------|---|-----------------------------------|
| Brownian force | $\vec{F}_{Brown} = \vec{\zeta} \sqrt{\frac{6 \pi \mu k_B T d_p}{\Delta t C_c}}$ | $\sim 10^{-18}$ |
| Stokes drag force | $\vec{F}_D = 3 \pi \mu_f d_p \vec{u}_r C_c^{-1}$ | $\sim 10^{-18}$ |

$$\vec{F} = m \cdot \vec{a}$$

$$m_p \frac{d^2 \vec{x}}{dt^2} = \vec{\zeta} \sqrt{\frac{6\pi\mu k_B T d_p}{\Delta t C_c}} + \frac{3\pi\mu_f d_p \vec{u}_r}{C_c}$$

Brownian force

Stokes drag force

ρ : density

T : temperature

$\vec{\zeta}$: vector of random numbers \vec{u}_r : relative particle velocity

\vec{x} : particle position

d_p : particle diameter

μ_f : fluid viscosity

k_B : Boltzmann constant

C_C : Cunningham slip corrector

C_C : Cunningham slip corrector

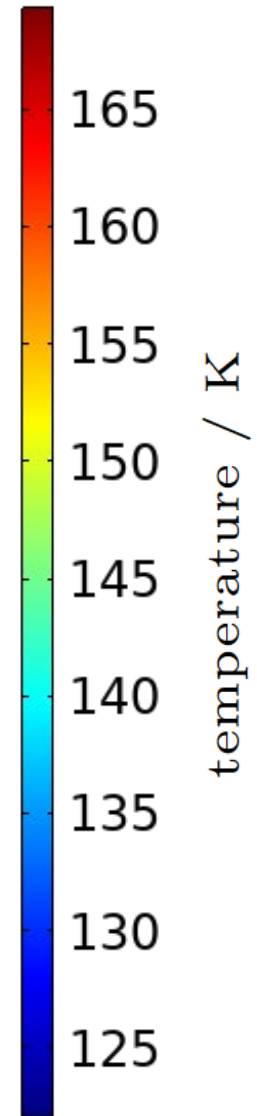
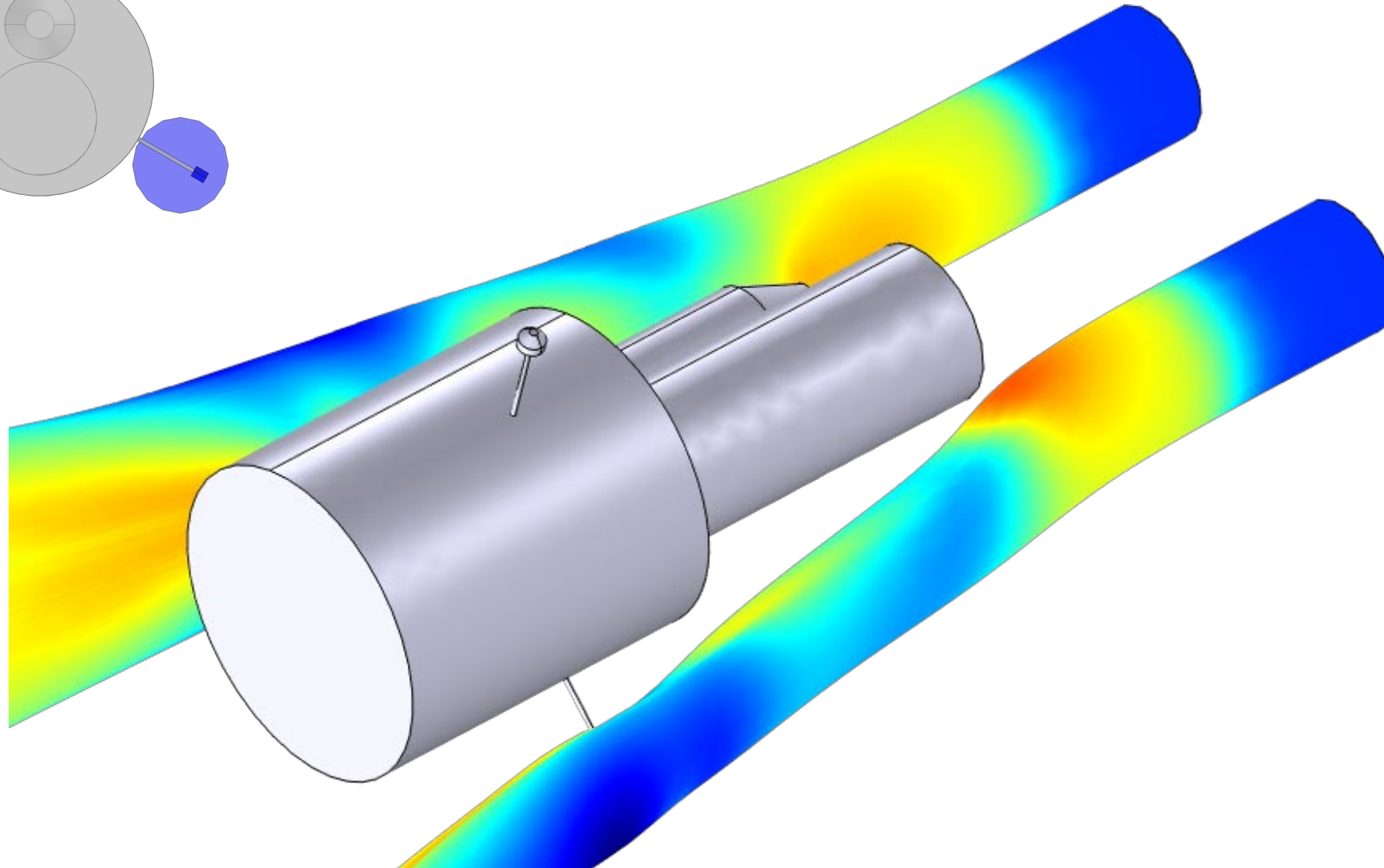
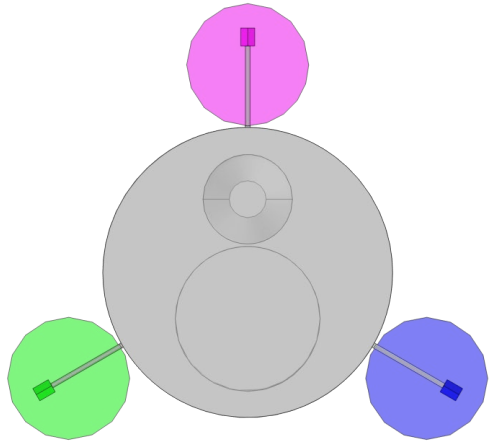
Particle calculations

| particle numbers | particle concentration [cm ⁻³] |
|------------------|--|
| 168 000 | 1 |
| 1 680 000 | 11 |
| 2 520 000 | 17 |
| 3 700 000 | 25 |
| 5 700 000 | 38 |

- Comsol implemented generalized α -method
- Parametric sweep
- Total solving time: ~3 days

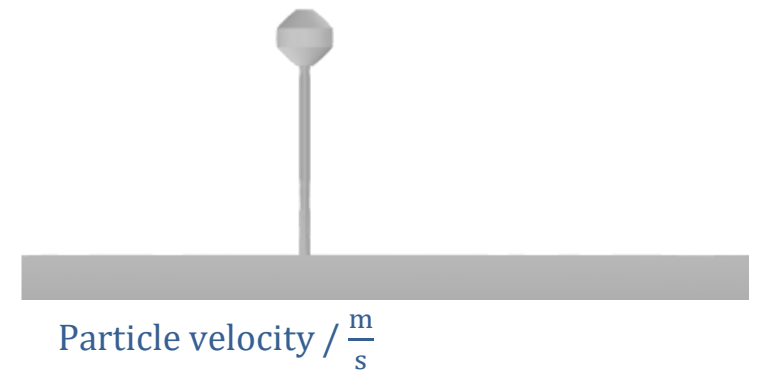
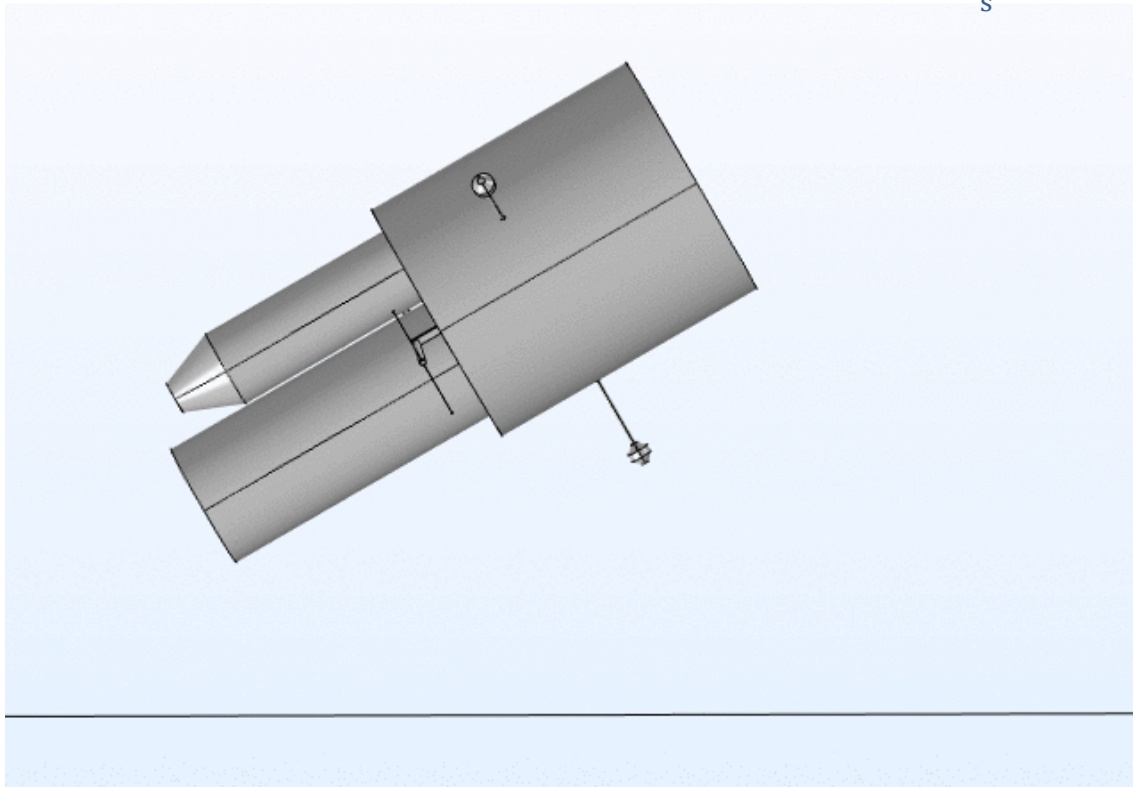
Simulation setup and results of particle calculations

Particle simulations

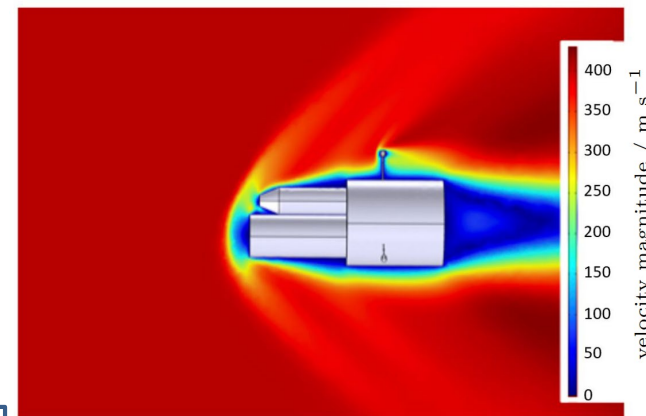
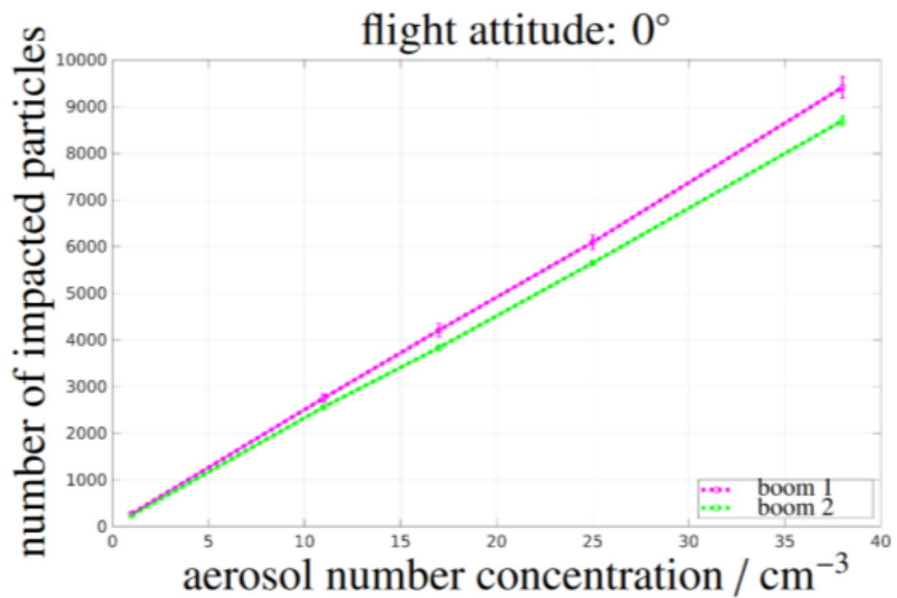


Particle simulation

Particle velocity / $\frac{m}{s}$

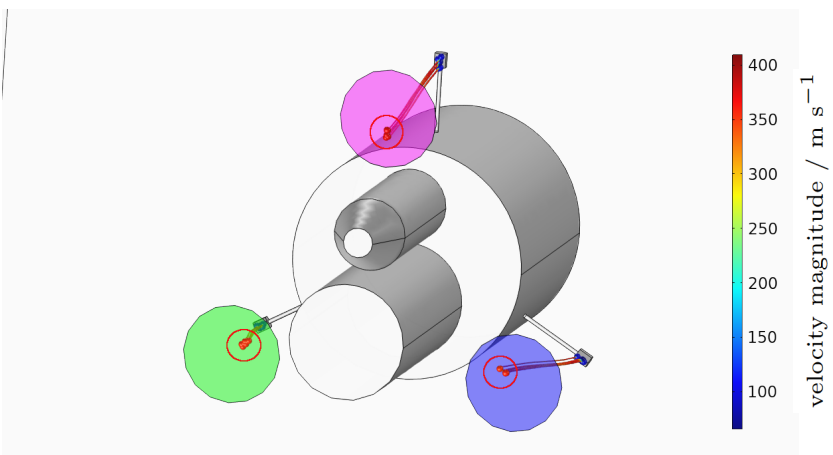
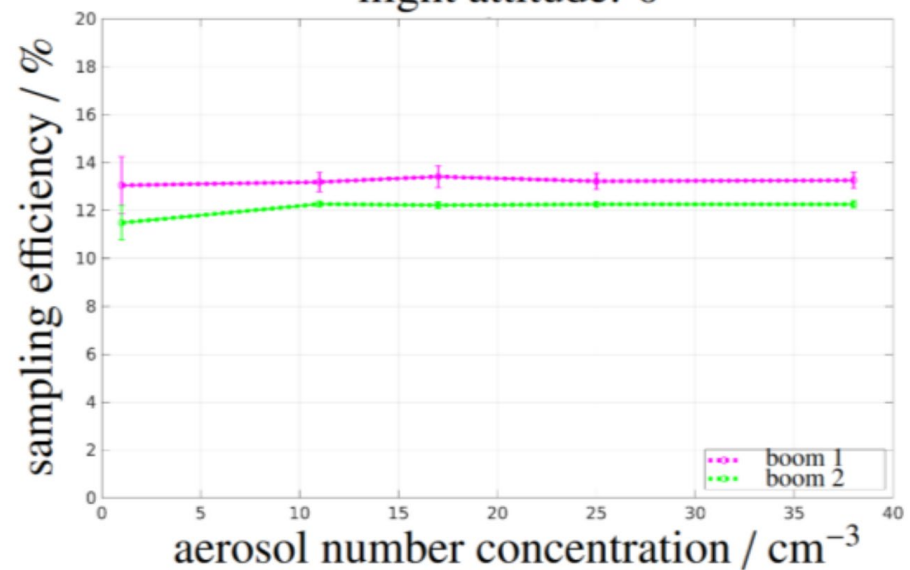


Particle simulation results



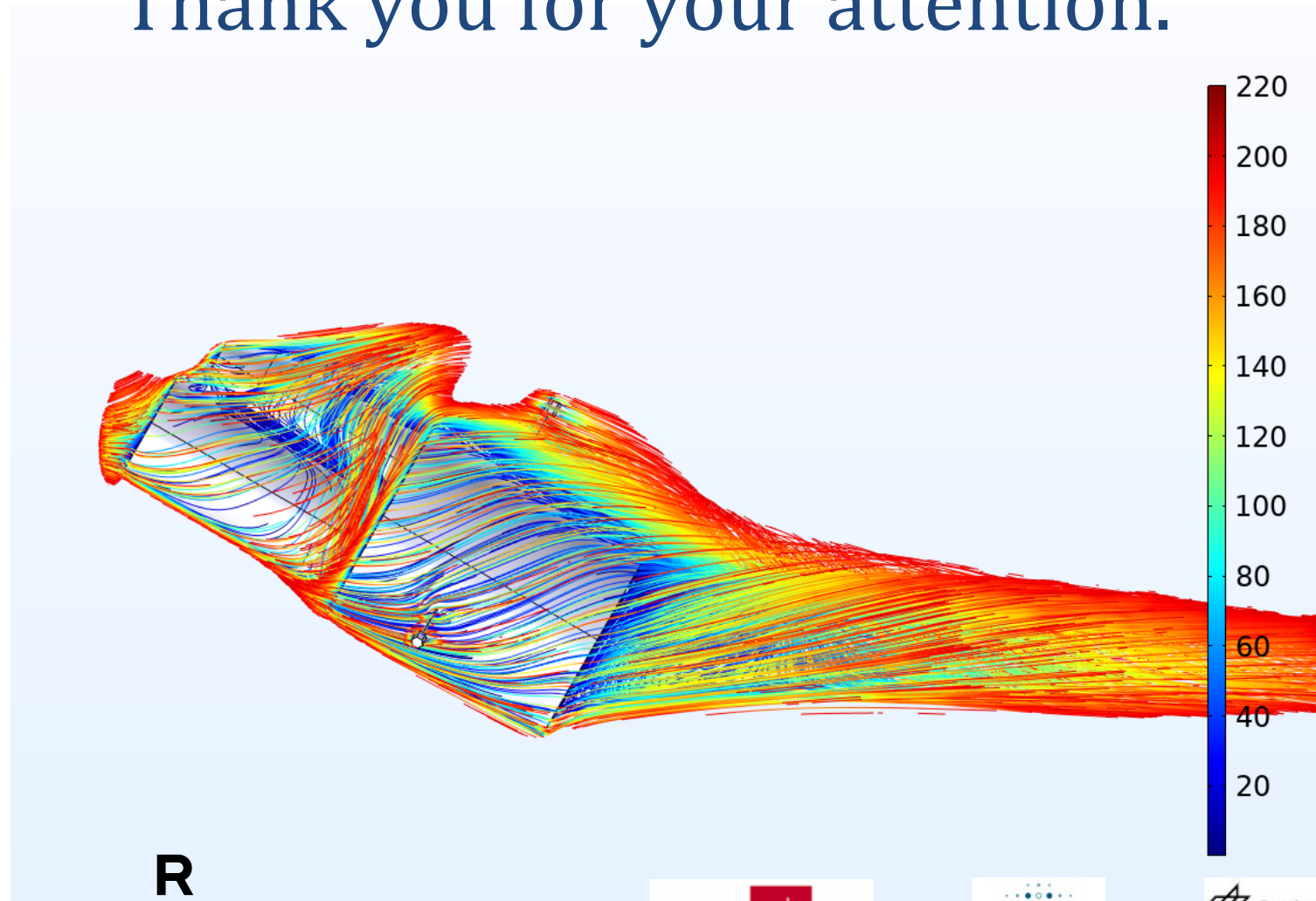
$$\text{efficiency} = \frac{C_{\text{impacted}}}{C_{\text{released}}}$$

flight attitude: 0°



Thank you for your attention.

Birte Klug
b.klug@rptu.de



Background

The solar system is full of dust

- collisions of asteroids
- sublimation of comets (dust-laden ice) orbiting the sun
 - dust trails
 - origin of meteor showers
- long-decayed cometary trails

(Plane, Chem. Soc. Rev., 2012, 41, 6507–6518)



What is the cosmic dust input to Earth's atmosphere?



Meteoric ablation

Interplanetary dust particles:

$3 - 300 \frac{t}{d}$

Peak ablation
~ 90 km

meteoric ablation

Meteoric Smoke
Particles

(Plane, Chem. Soc. Rev., 2012, 41, 6507–6518)

Noctilucent Clouds (NLC)



© Philipp Reutter

Philipp Reutter, 05 Jul 2020, Sulzheim

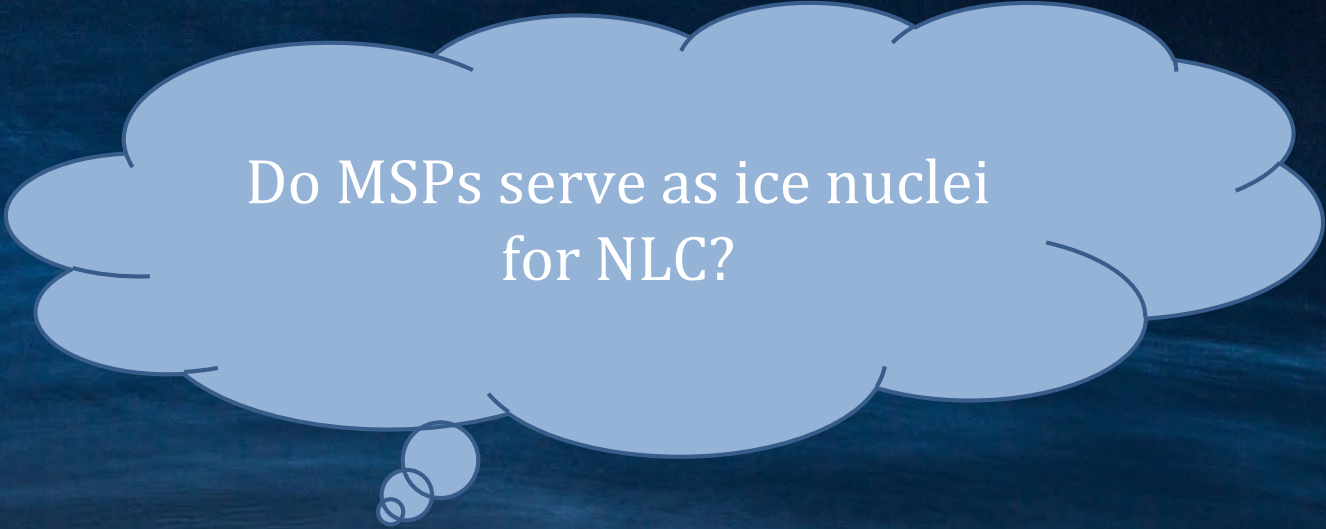
Noctilucent Clouds (NLC)

Cirrus like
structure

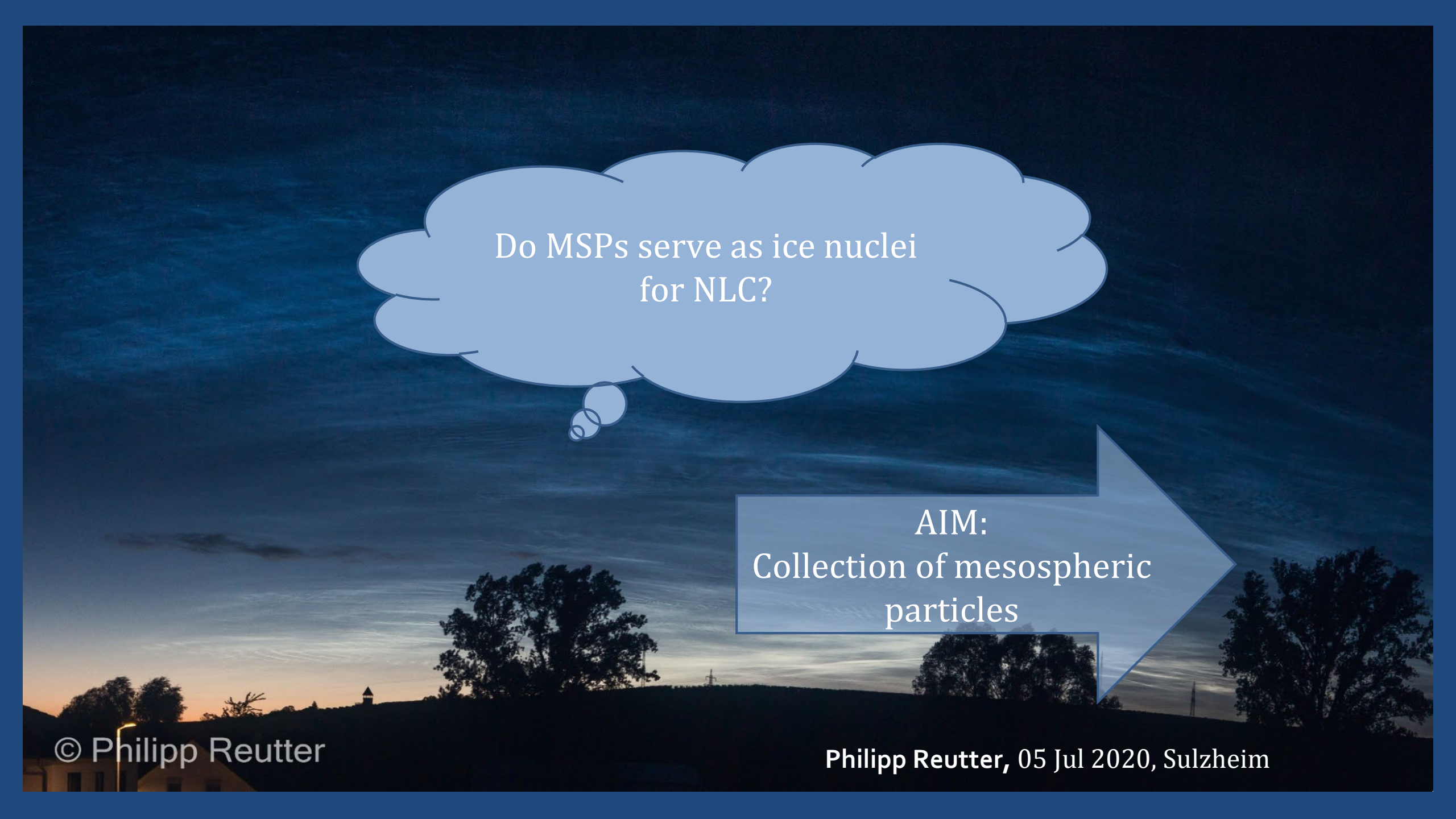
82 – 85 km

Ice particles

Polar summer
mesopause

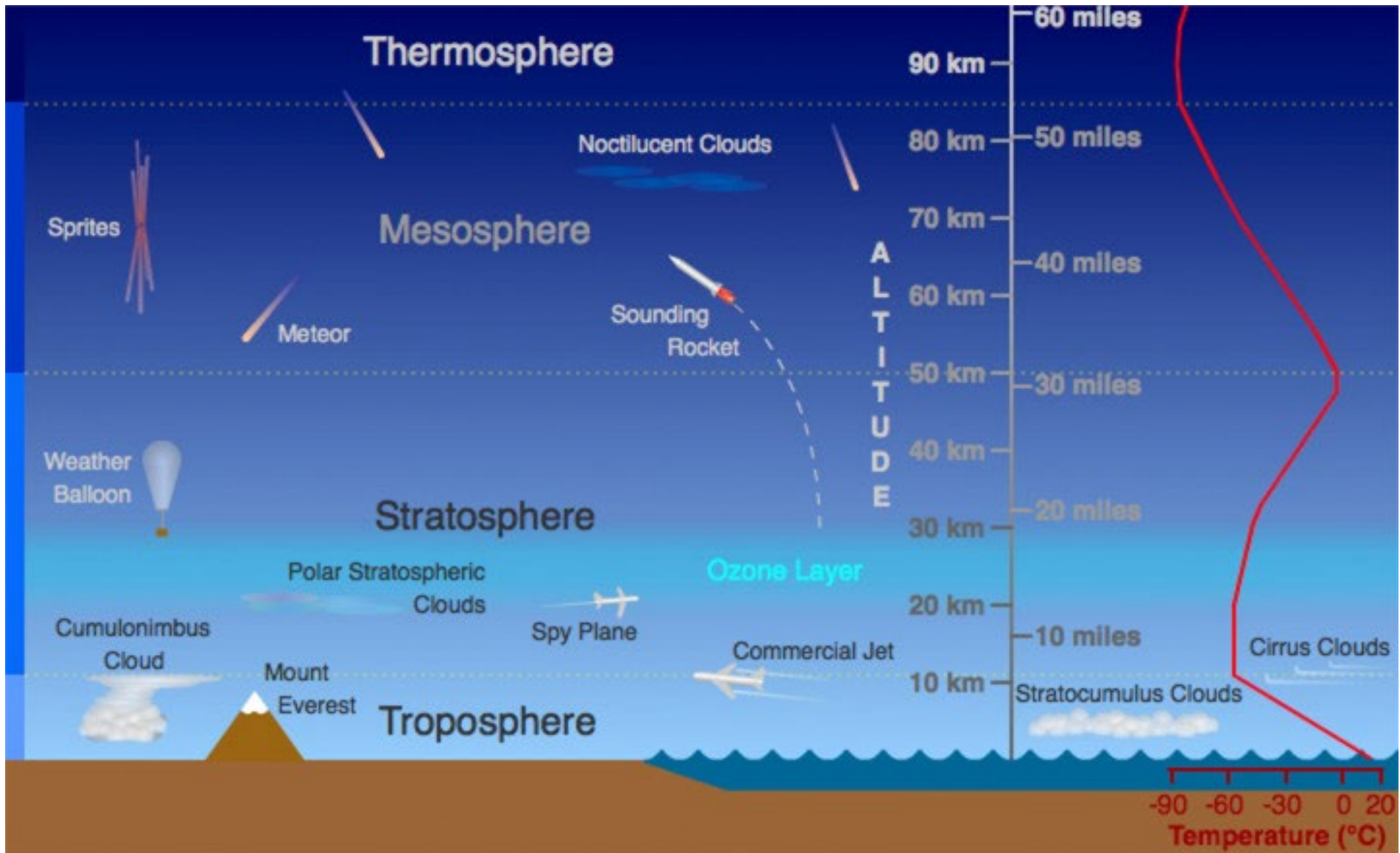


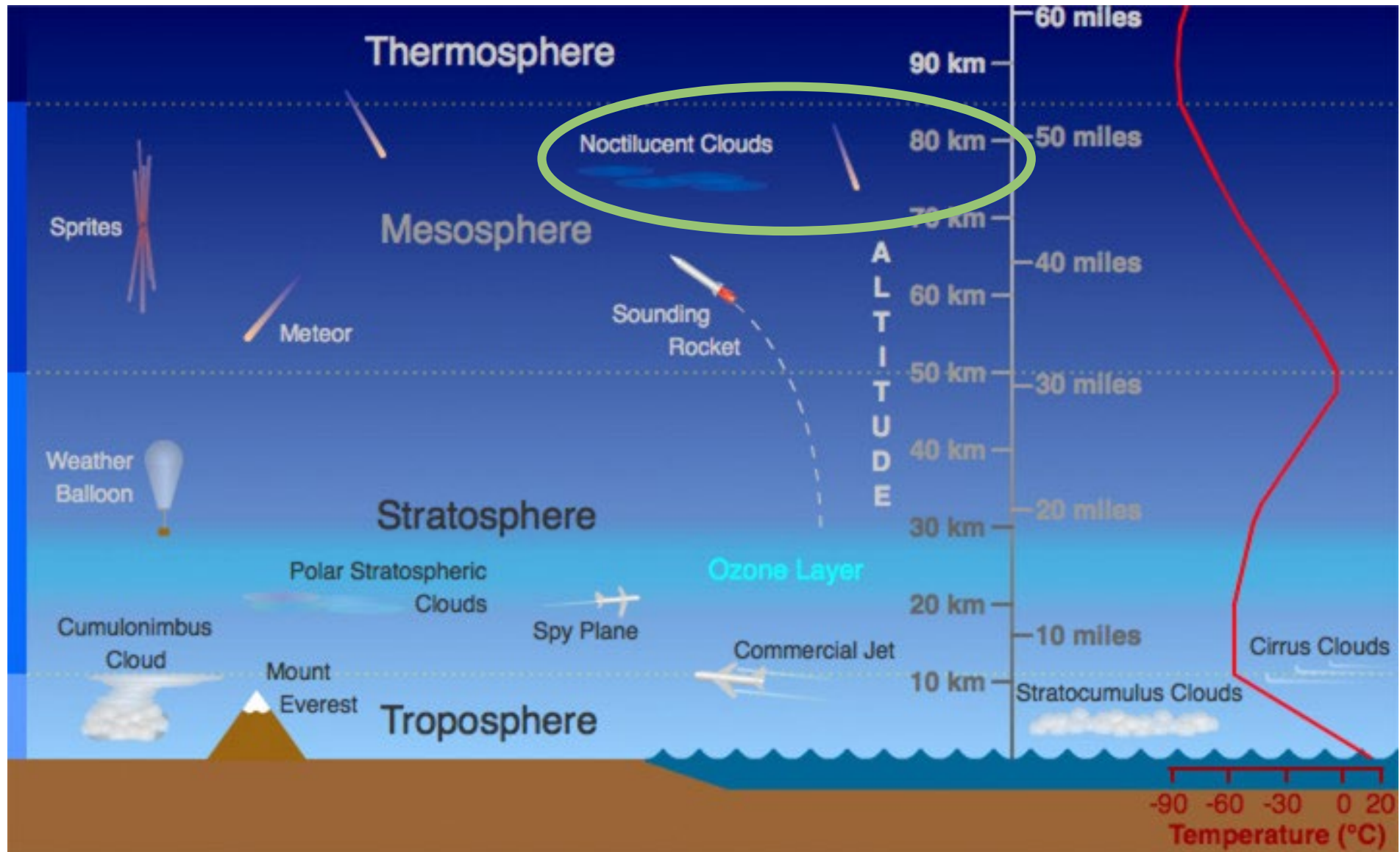
Do MSPs serve as ice nuclei
for NLC?



Do MSPs serve as ice nuclei
for NLC?

AIM:
Collection of mesospheric
particles







The solar system is full of dust

What is the origin of cosmic dust?



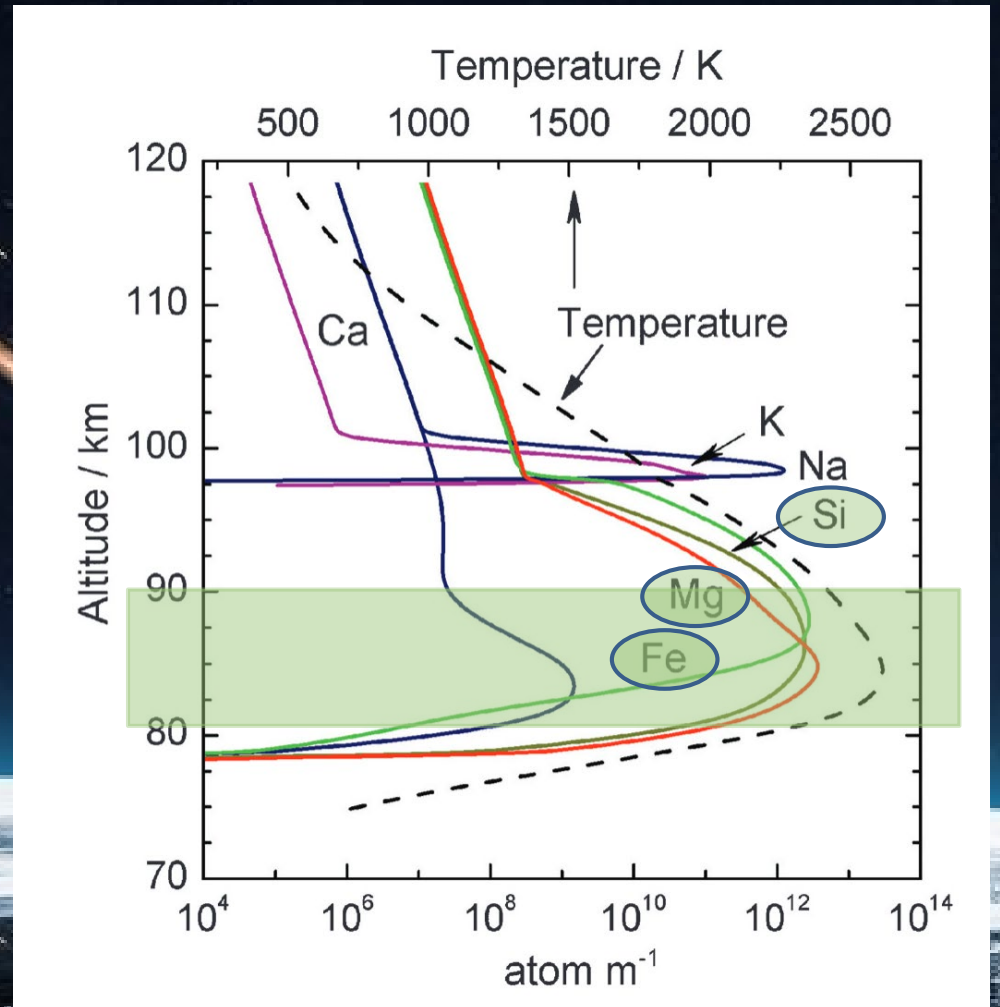
The solar system is full of dust

Main sources of dust particles:

- collisions of asteroids
- sublimation of comets (dust-laden ice) orbiting the sun
 - dust trails
 - origin of meteor showers
- long-decayed cometary trails

(Plane, Chem. Soc. Rev., 2012, 41, 6507–6518)

Meteoric ablation

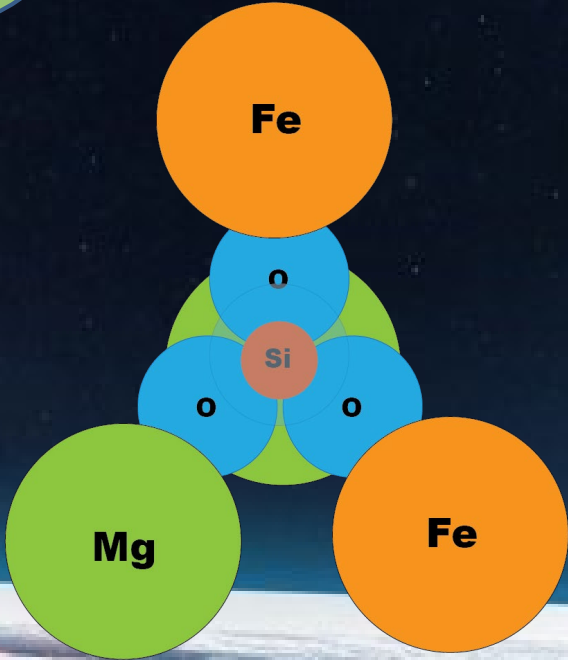


(Plane, Chem. Soc. Rev., 2012, 41, 6507–6518)

Meteoric ablation



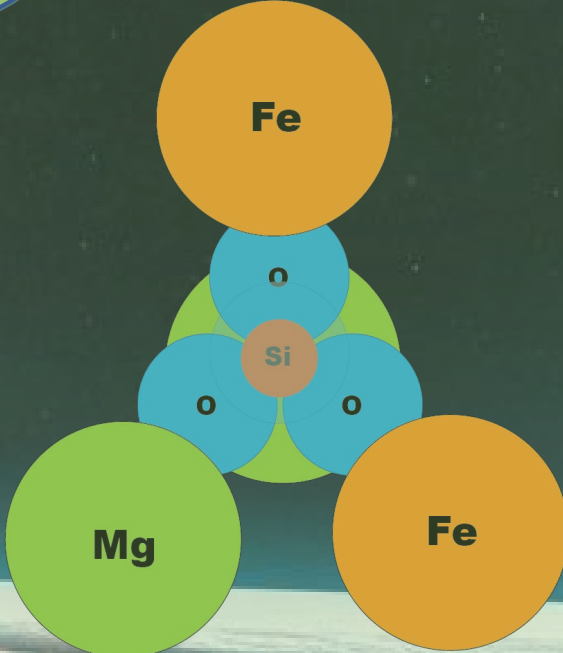
Olivine-like
 Fe-Mg-SiO_4



Meteoric ablation

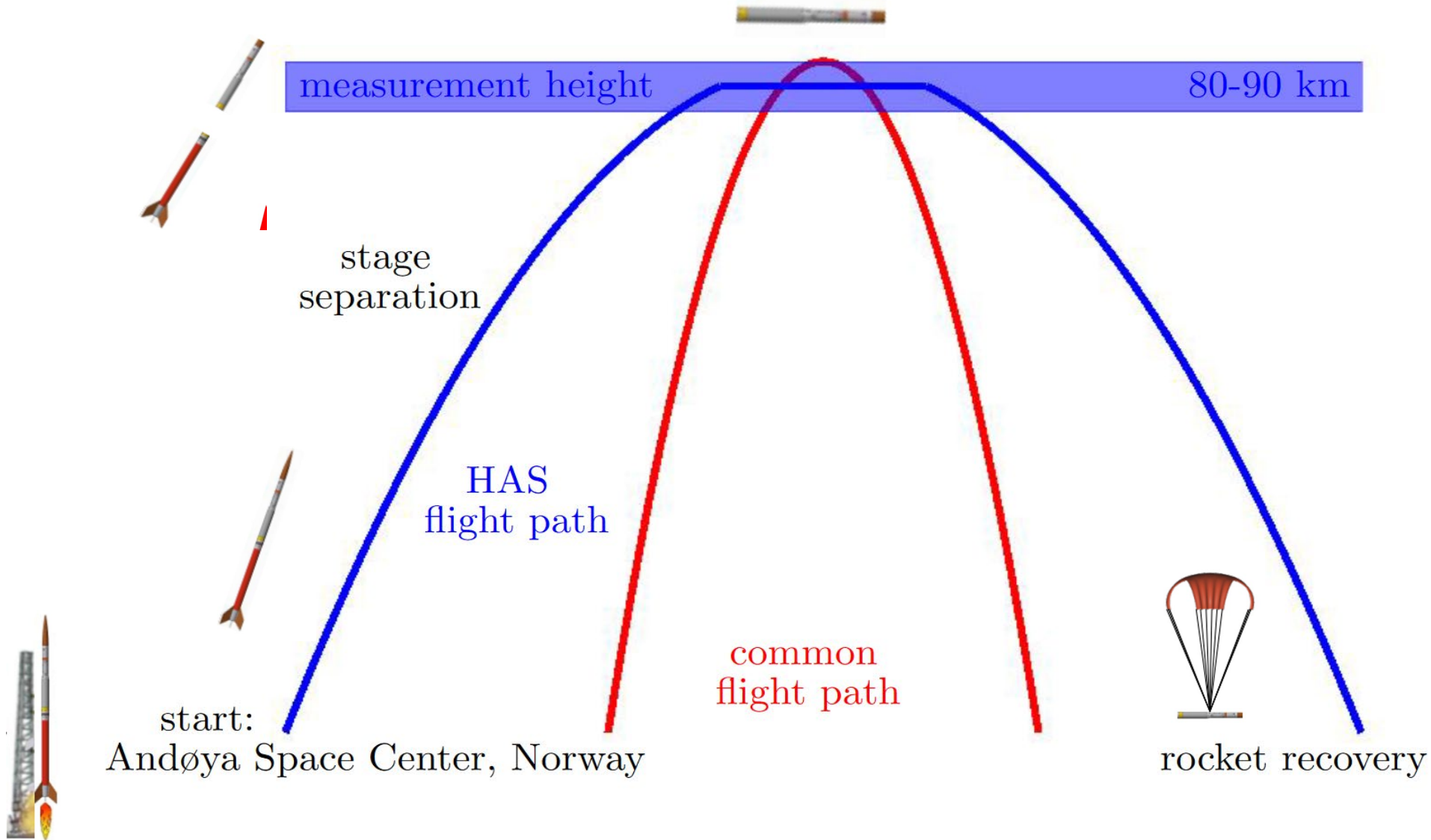


Olivine-like
 Fe-Mg-SiO_4

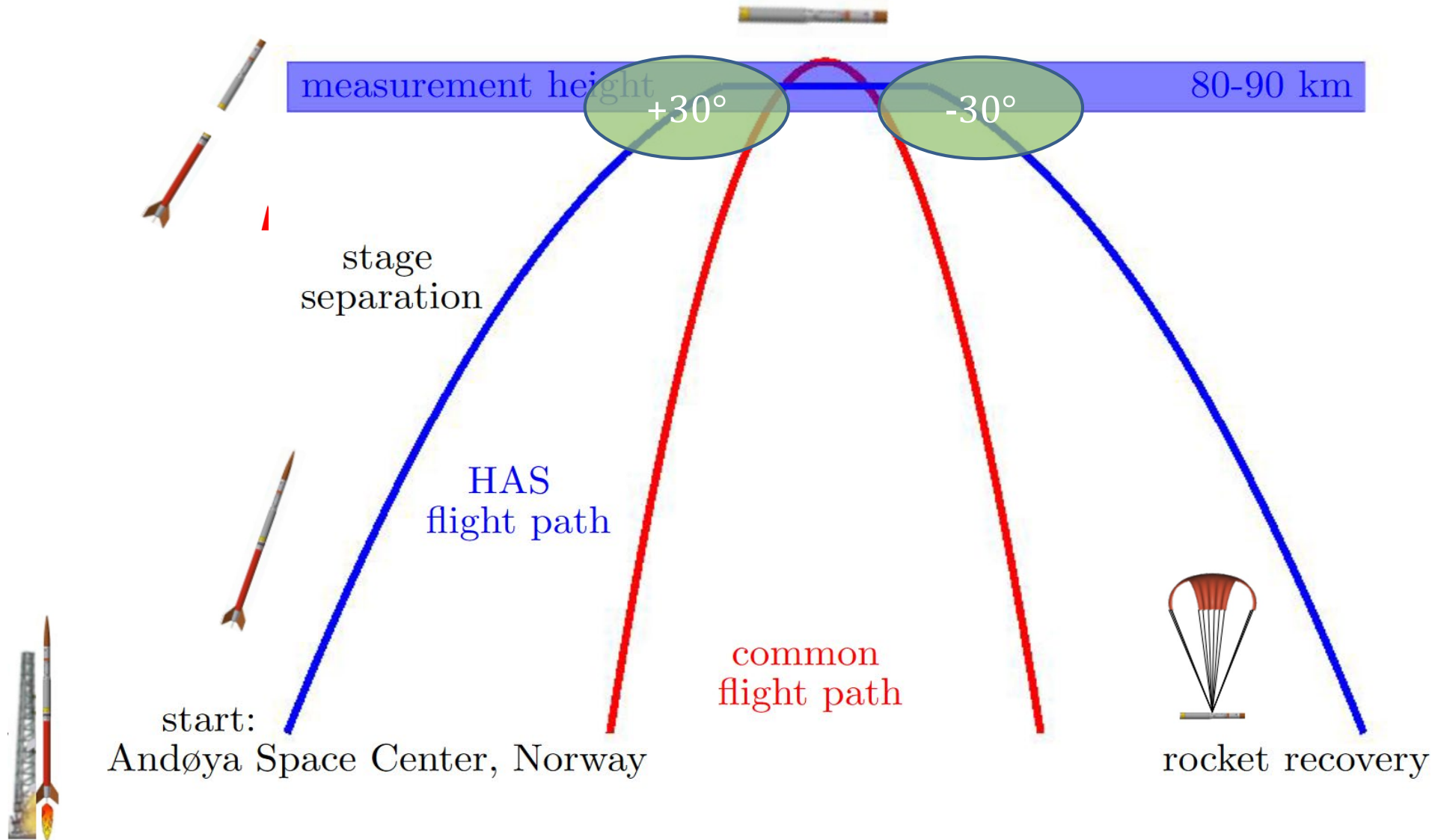


Meteoric Smoke Particles (MSP)

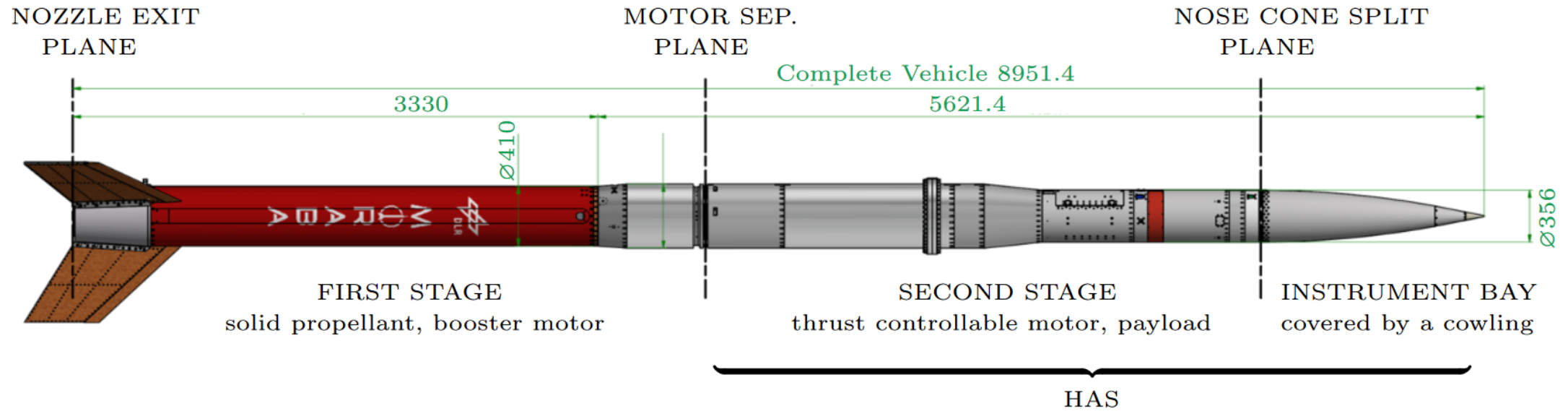
Flight path of the rocket



Flight path of the sounding rocket

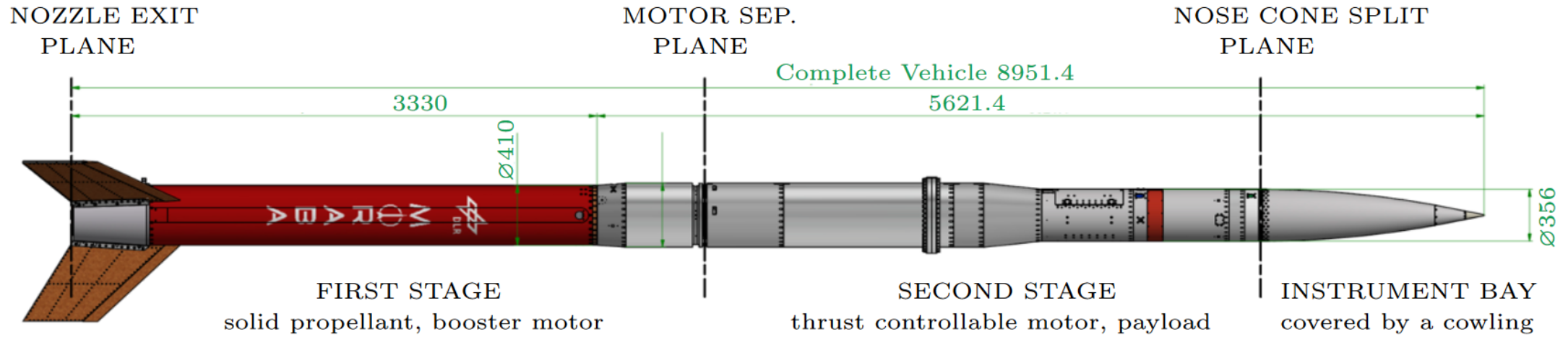


Sounding rocket

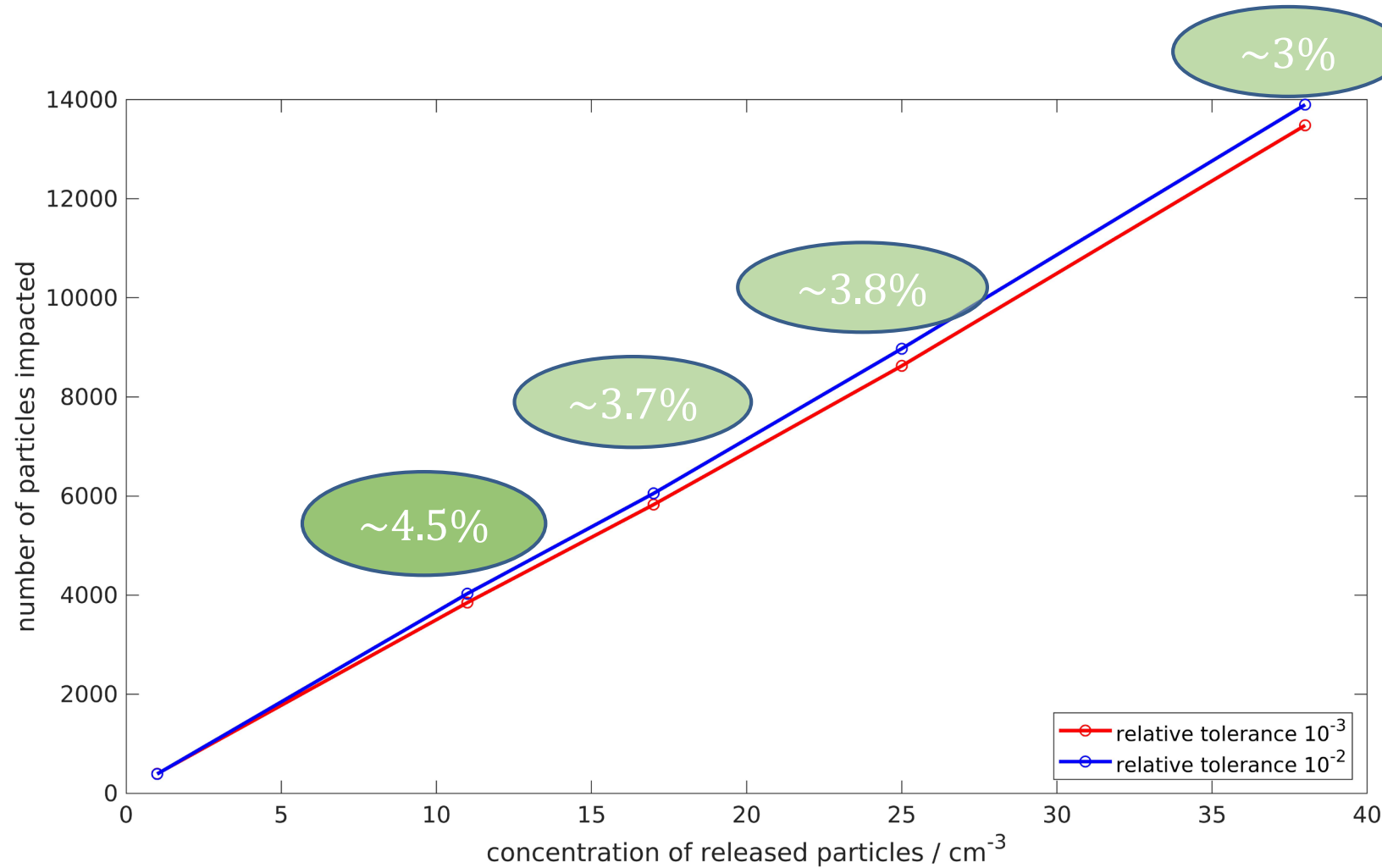


thrust controllable
experiment carrier

DLR-
Moraba



Particle simulations



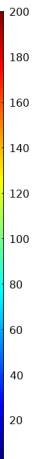
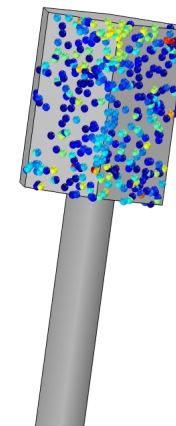
Relative tolerance Tol

$Tol = 10^{-3}$ with $\Delta t \sim 3 \cdot 10^{-6}$ s

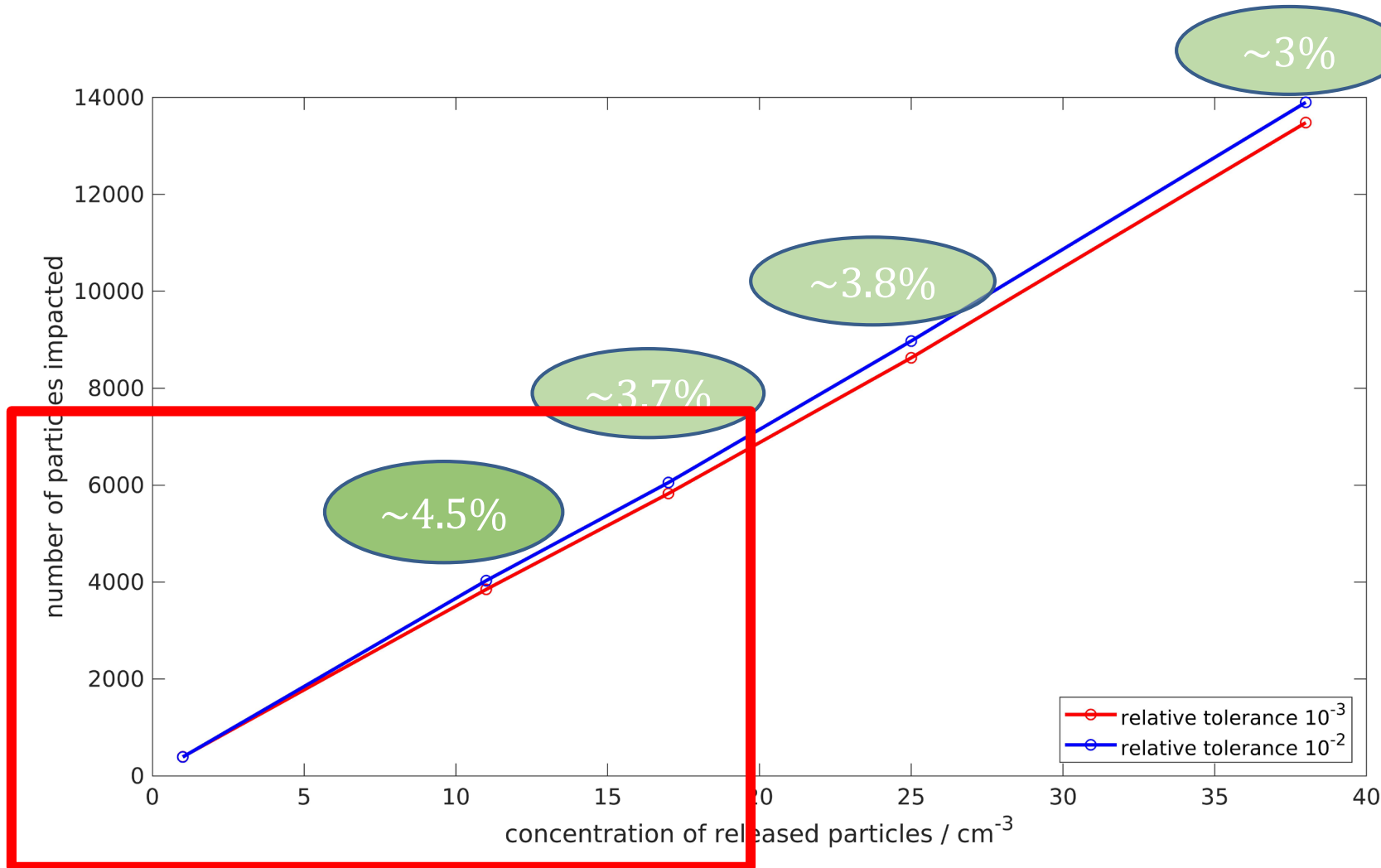
Simulation time: ~ 90 h

$Tol = 10^{-2}$ with $\Delta t \sim 2 \cdot 10^{-5}$ s

Simulation time: ~ 30 h



Particle simulations



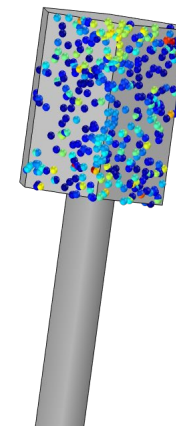
Relative tolerance Tol

$Tol = 10^{-3}$ with $\Delta t \sim 3 \cdot 10^{-6}$ s

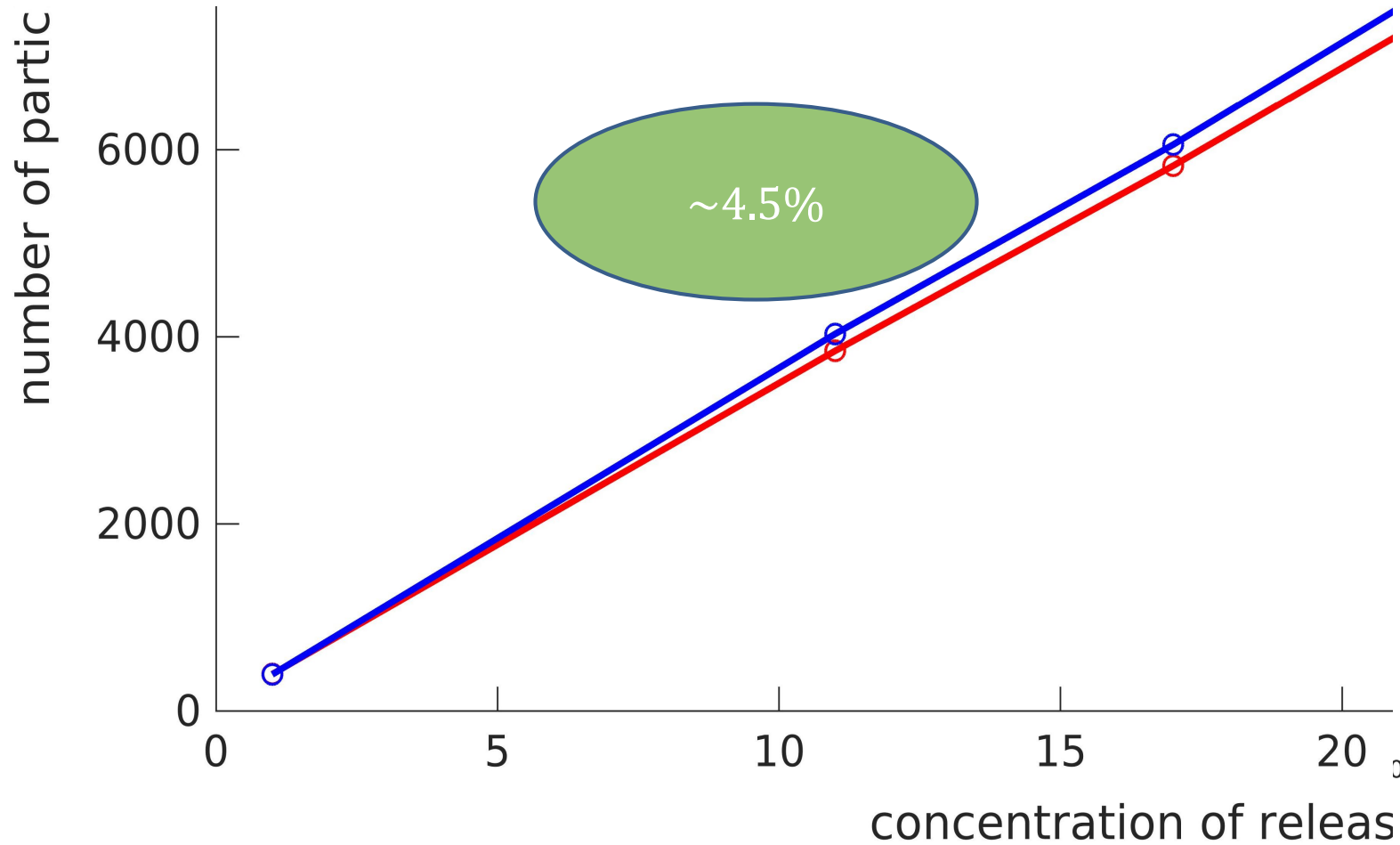
Simulation time: ~ 90 h

$Tol = 10^{-2}$ with $\Delta t \sim 2 \cdot 10^{-5}$ s

Simulation time: ~ 30 h



Particle simulations



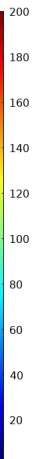
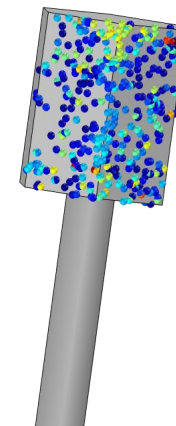
Relative tolerance Tol

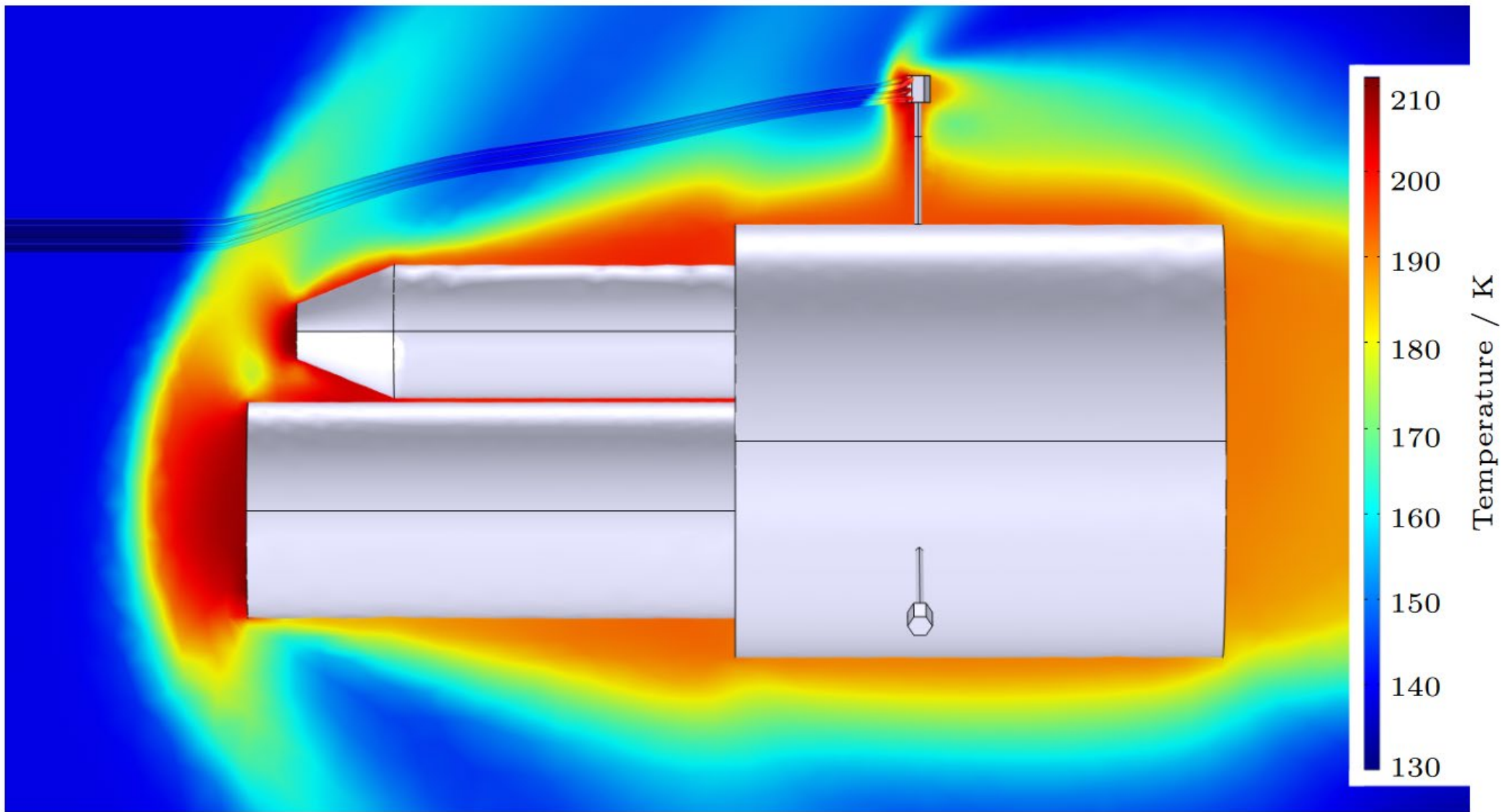
$Tol = 10^{-3}$ with $\Delta t \sim 3 \cdot 10^{-6}$ s

Simulation time: ~ 90 h

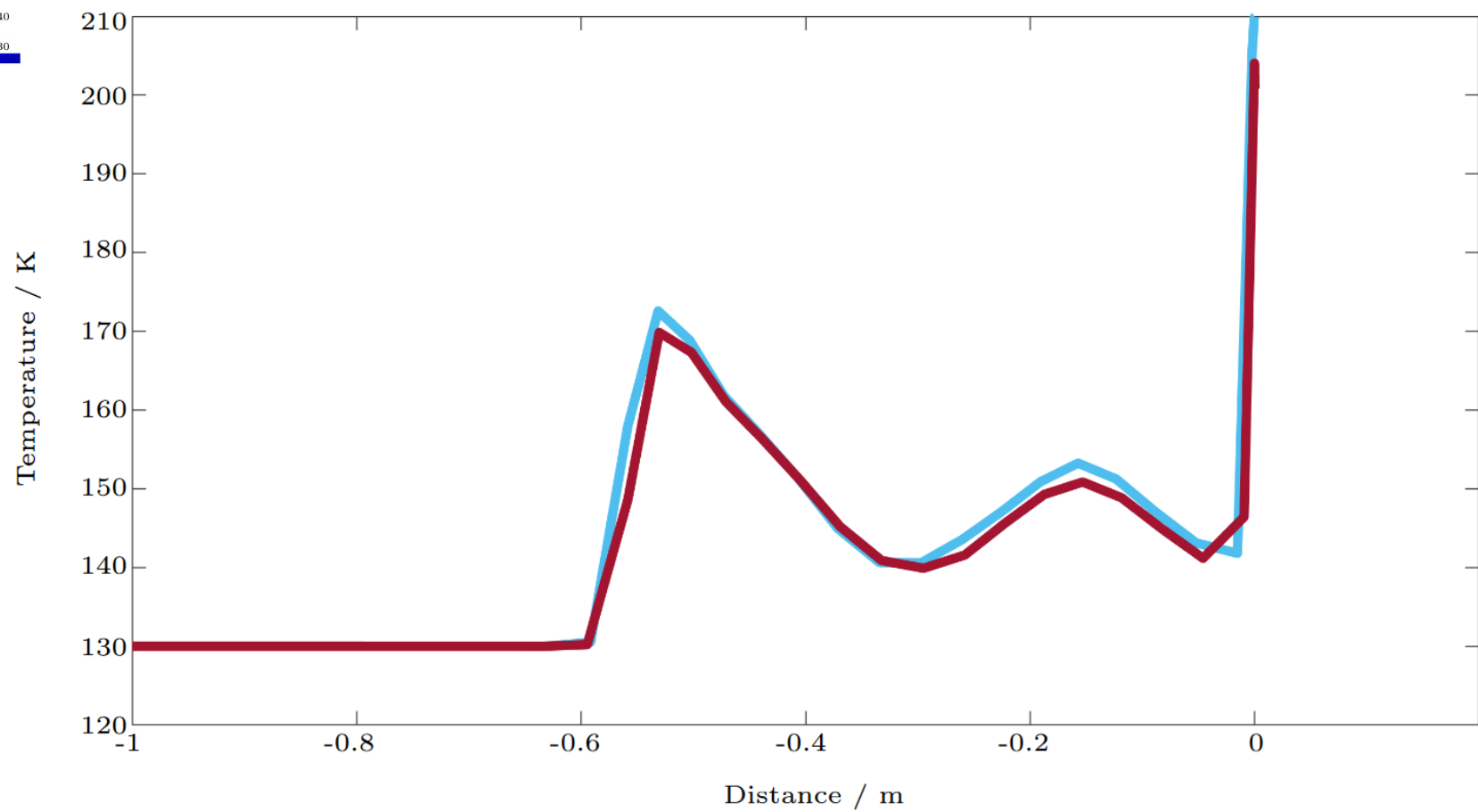
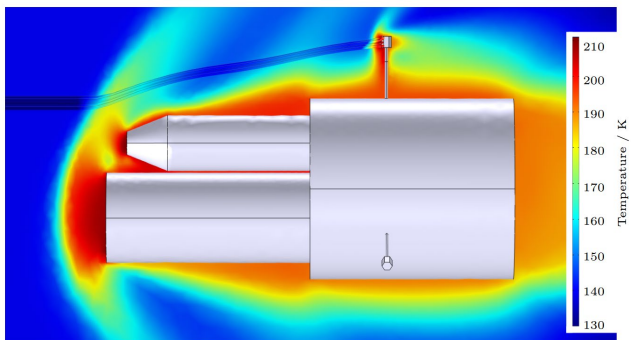
$Tol = 10^{-2}$ with $\Delta t \sim 2 \cdot 10^{-5}$ s

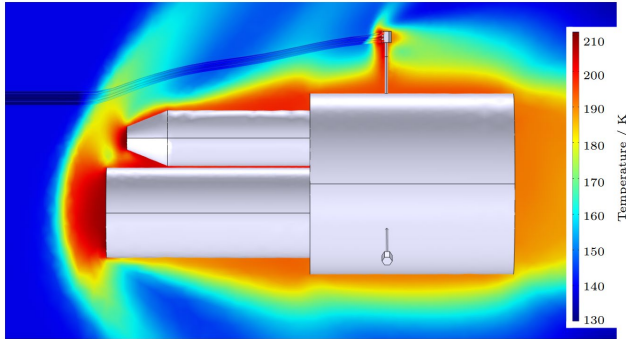
Simulation time: ~ 30 h



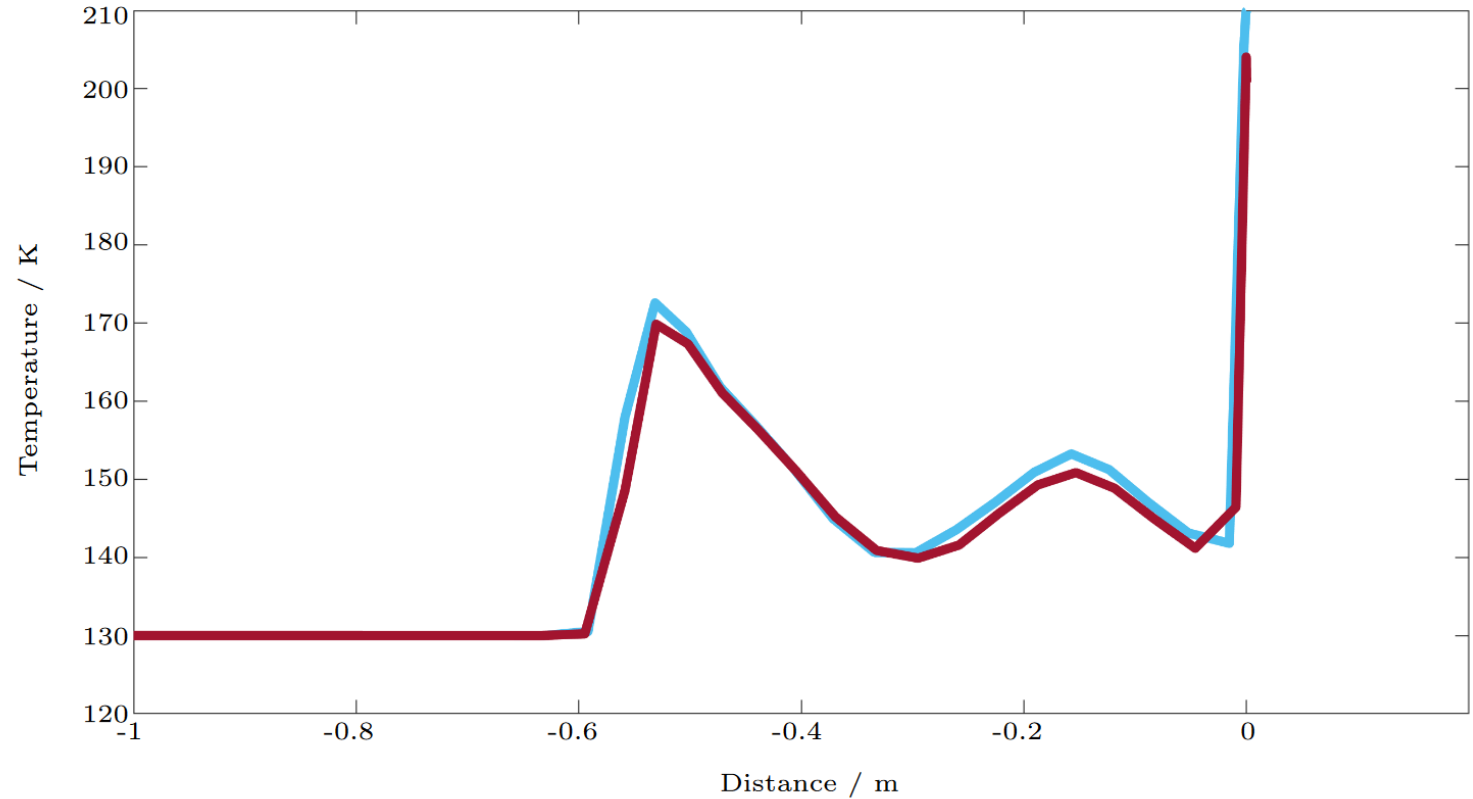


Temperature field in K depicted on a cut plane and particle trajectories





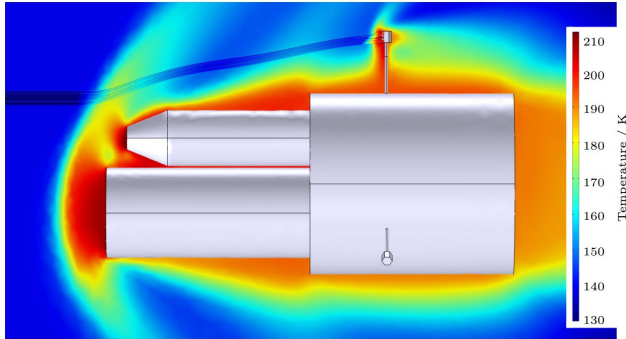
$$\frac{dm_{ice}}{dt} = \frac{4\pi}{R_v} \alpha_d D_v r \left(\frac{p}{T_{air}} - \frac{p}{T_{ice}} \right)$$



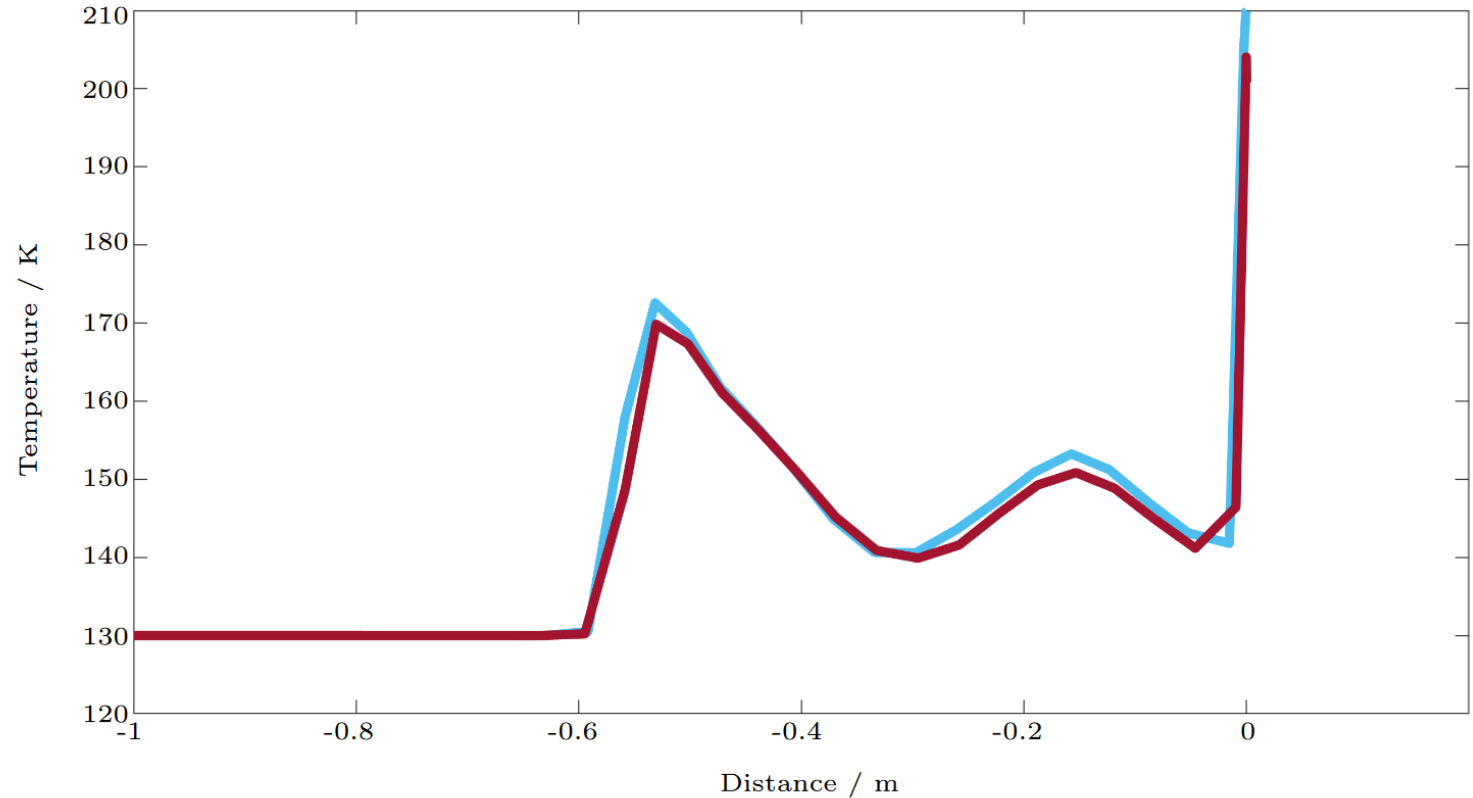
D_v : diffusion coefficient of water vapor in air
 p : pressure
 r : particle radius

T_{air} : ambient temperature
 T_{ice} : surface temperature
 α_d : deposition coefficient

R_v : water vapor gas constant
 p : pressure
 r : particle radius



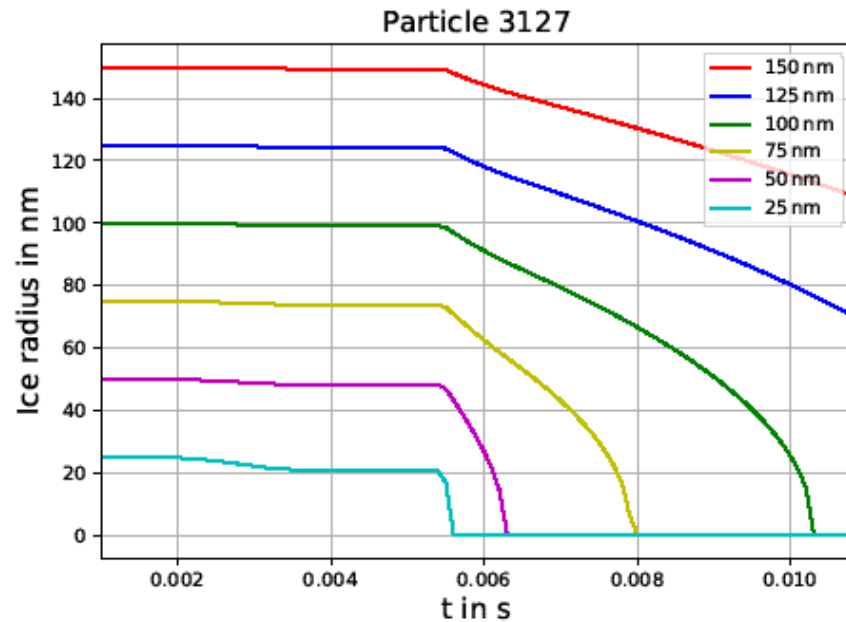
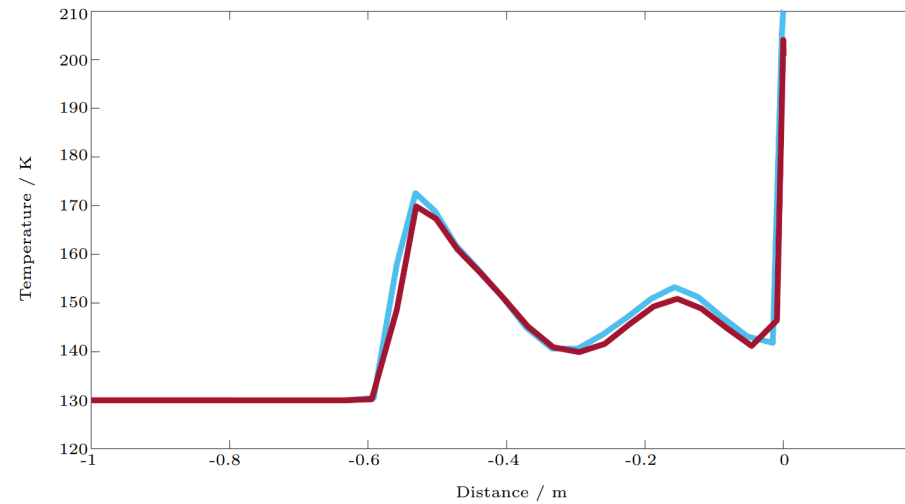
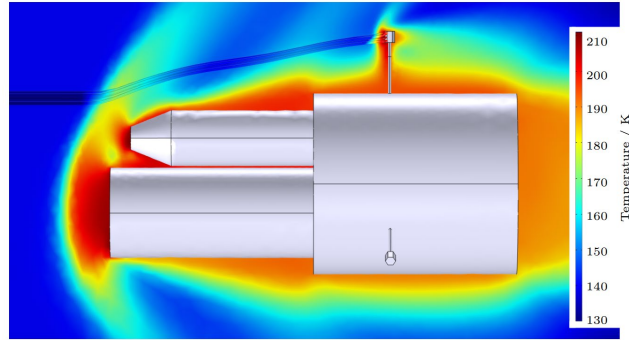
$$\frac{dm_{ice}}{dt} = \frac{4\pi}{R_v} \alpha_d D_v r \left(\frac{p}{T_{air}} - \frac{p}{T_{ice}} \right)$$



D_v : diffusion coefficient of water vapor in air
 p : pressure
 r : particle radius

T_{air} : ambient temperature
 T_{ice} : surface temperature
 α_d : deposition coefficient

R_v : water vapor gas constant
 p : pressure
 r : particle radius

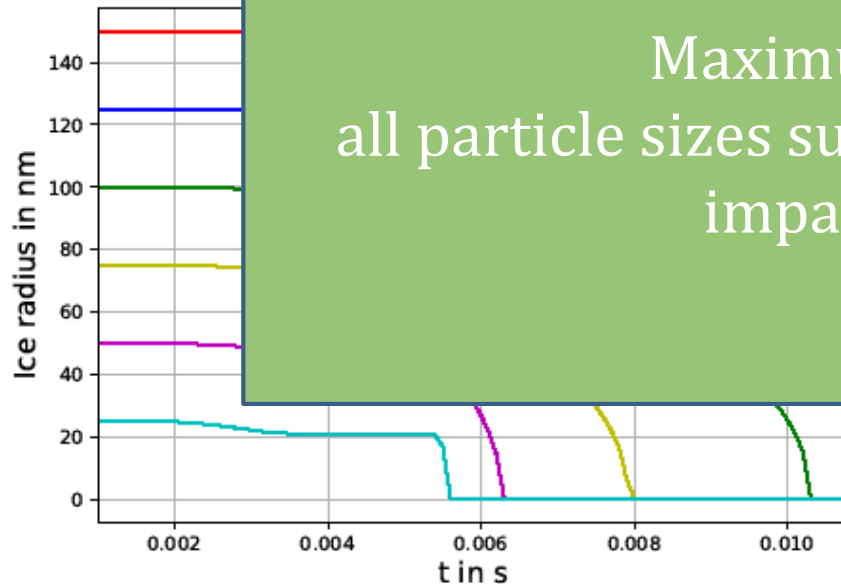
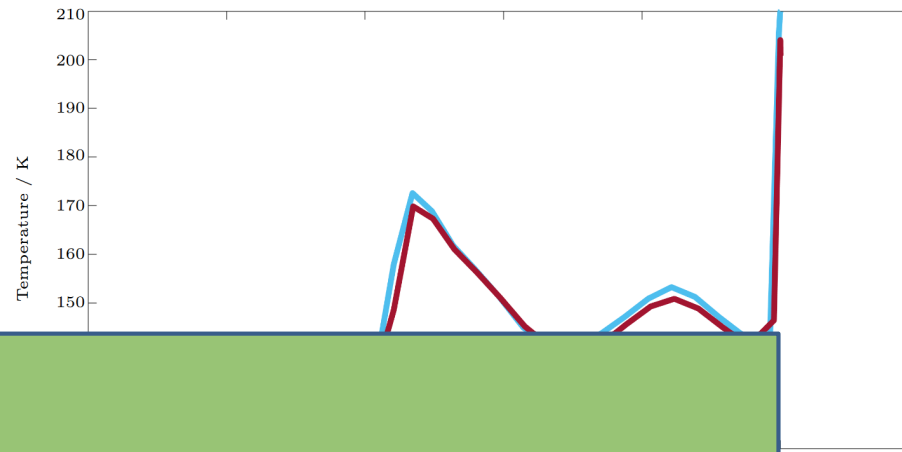
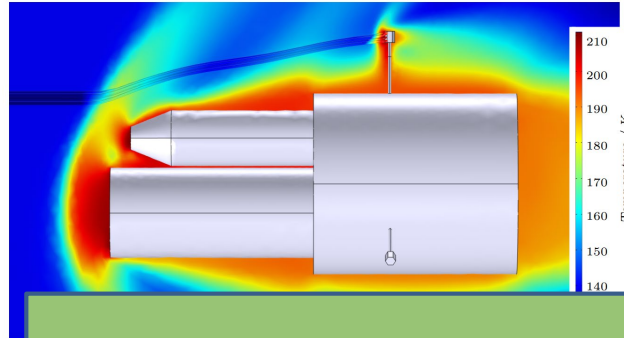


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Maximum assumption:
all particle sizes sublime on their way to the
impaction surfaces

$$\left(\frac{p}{T_{air}} - \frac{p}{T_{ice}} \right)$$

D_v : diffusion coefficient of water vapor in air
 p : pressure
 r : particle radius

T_{air} : ambient temperature
 T_{ice} : surface temperature
 α_d : deposition coefficient

R_v : water vapor gas constant
 p : pressure
 r : particle radius

Particle data

NLC particle
 $\rho_p = 1 \frac{\text{g}}{\text{cm}^3}$

$r_p \leq 10 \mu\text{m}$

$C=1-10 \text{ cm}^{-3}$

Turco et al., Planetary and Space Science, 30:1147-1181, 1982.

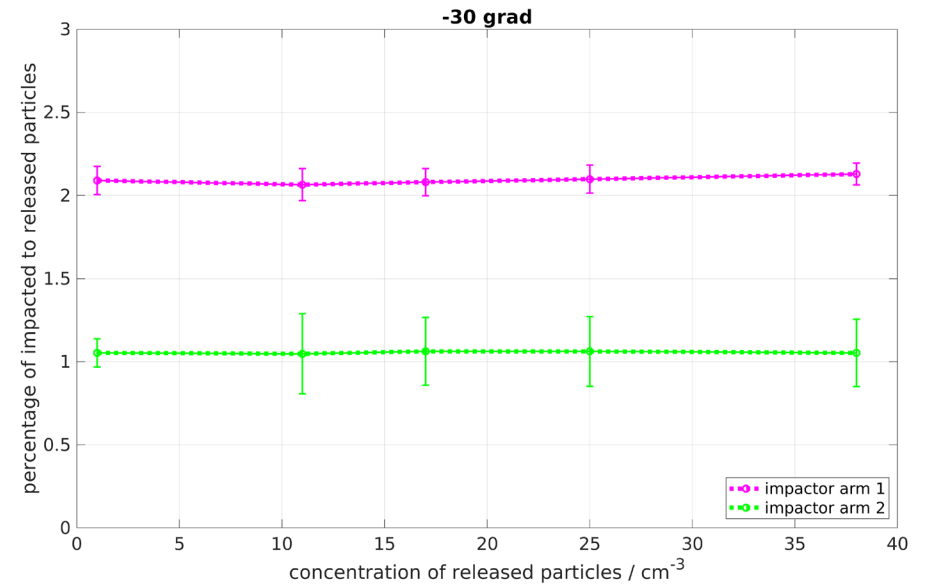
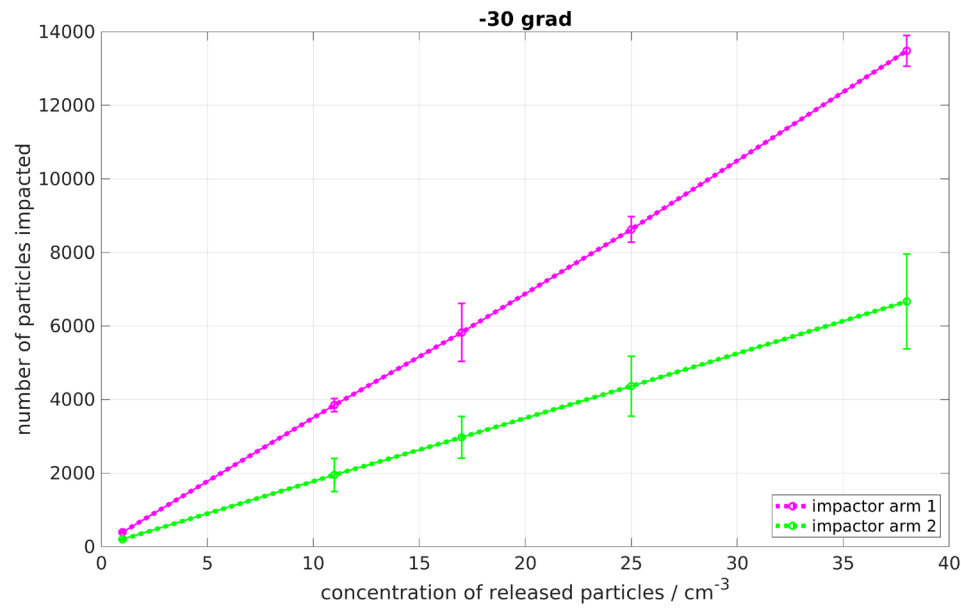
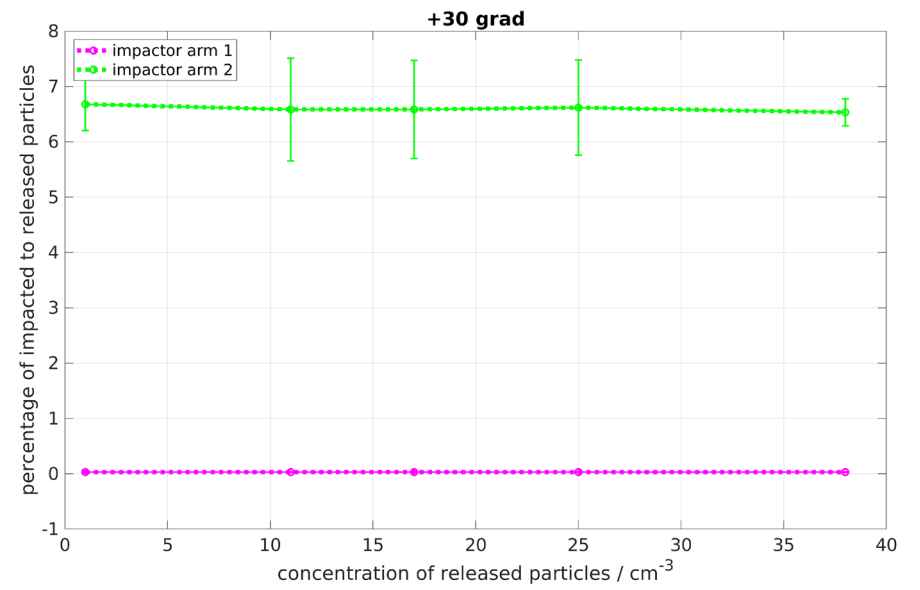
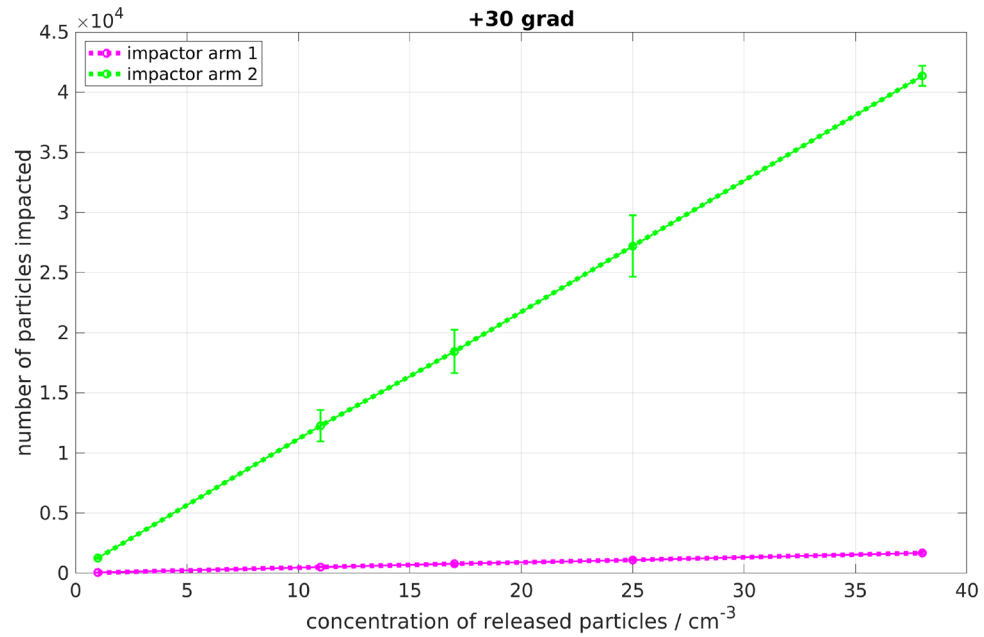
MSP particle
 $\rho_{MSP} = 3 \frac{\text{g}}{\text{cm}^3}$

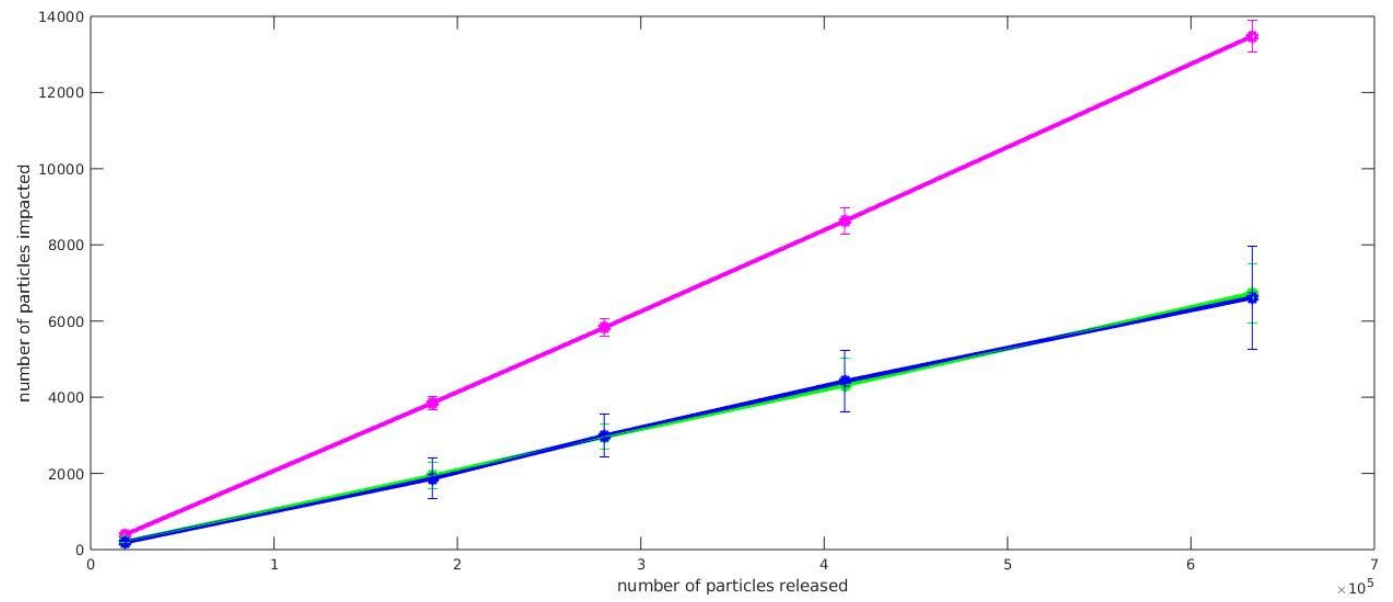
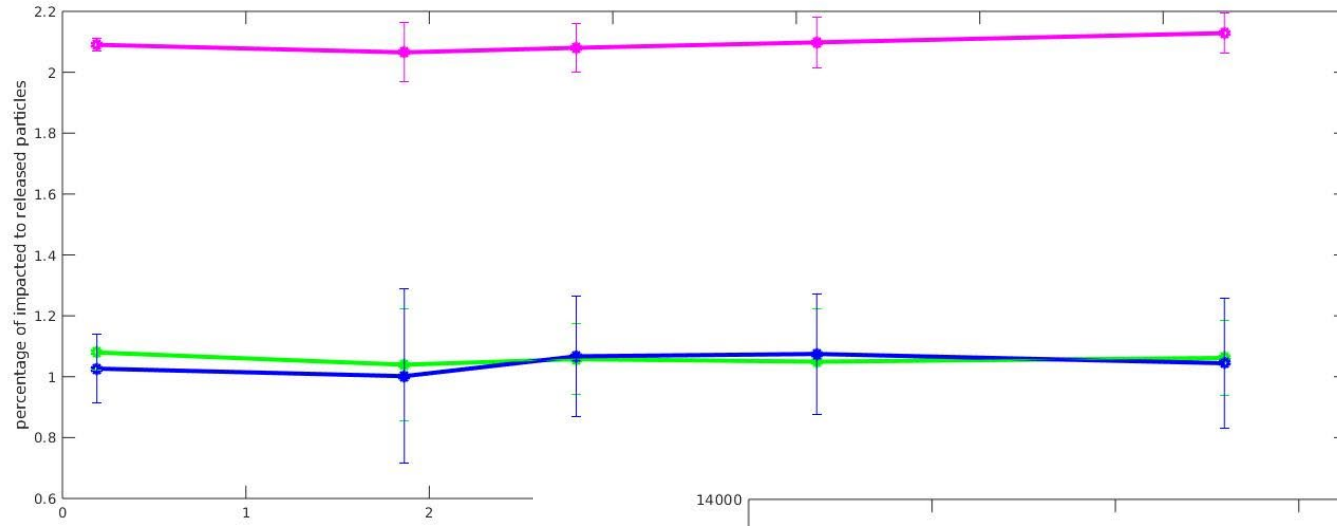
$r_{MSP} = 0.4 - 0.8 \text{ nm}$

Hedin et al., Journal of Atmospheric and Solar-Terrestrial Physics, 118:127-114, 2014.

| parameters | values | comments |
|---------------------------------------|--|---|
| ambient conditions | | |
| μ_f | $8.99847 \cdot 10^{-6} \text{ Pa s}$ | Dynamic viscosity of air at 85 km. |
| ρ_f | $2.6798 \cdot 10^{-5} \text{ kg m}^{-3}$ | Air density, model variable for the current situation at 85 km altitude. |
| m_f | $2.43 \cdot 10^{-32} \text{ kg}$ | Mass of fluid, displaced by a particle of $d_p = 1.2 \cdot 10^{-9} \text{ m}$. |
| $\frac{\partial u}{\partial y}$ | 650 s^{-1} | Velocity gradient estimated from numerical simulations. |
| $\frac{d(\vec{u}_f - \vec{v}_f)}{dt}$ | $1 \cdot 10^7 \text{ m s}^{-1}$ | Maximum relative particle acceleration (from numerical simulations for $\vec{u}_f = 300 \text{ m s}^{-1}$). |
| ∇p | 1.05 Pa m^{-1} | Pressure gradient (from numerical simulations). |
| k_B | $1.381 \cdot 10^{-23} \text{ J K}^{-1}$ | Boltzmann constant. |
| \vec{g} | 9.5 m s^{-2} | Gravitational acceleration coefficient at 85 km. |
| particle properties | | |
| $\vec{u}_r = \vec{u}_f - \vec{v}_p$ | 120 m s^{-1} | Maximum relative particle velocity (from numerical simulations for $\vec{u}_f = 300 \text{ m s}^{-1}$). |
| d_{pcd} | $100 \cdot 10^{-9} \text{ m}$ Rapp and Thomas [2006] | Diameter of a single cloud droplet. |
| ρ_{pcd} | 1000 kg m^{-3} | Density of a cloud droplet. |
| d_{psn} | $1.2 \cdot 10^{-9} \text{ m}$ Hedin et al., 2014] | Diameter of a single sublimation nuclei. |
| ρ_{psn} | 3000 kg m^{-3} Hedin et al., 2007] | Density of a sublimation nuclei. |
| m_p | $2.7 \cdot 10^{-24} \text{ kg}$ | Mass of a single particle for $d_p = 1.2 \cdot 10^{-9} \text{ m}$ and $\rho = 3000 \text{ kg m}^{-3}$. |
| C_c | $7.357 \cdot 10^4$ | Cunningham slip corrector for particles with $d_p = 1.2 \cdot 10^{-9} \text{ m}$. |
| simulation data | | |
| Δt | $1 \cdot 10^{-5}$ | Example time step taken by the solver. |

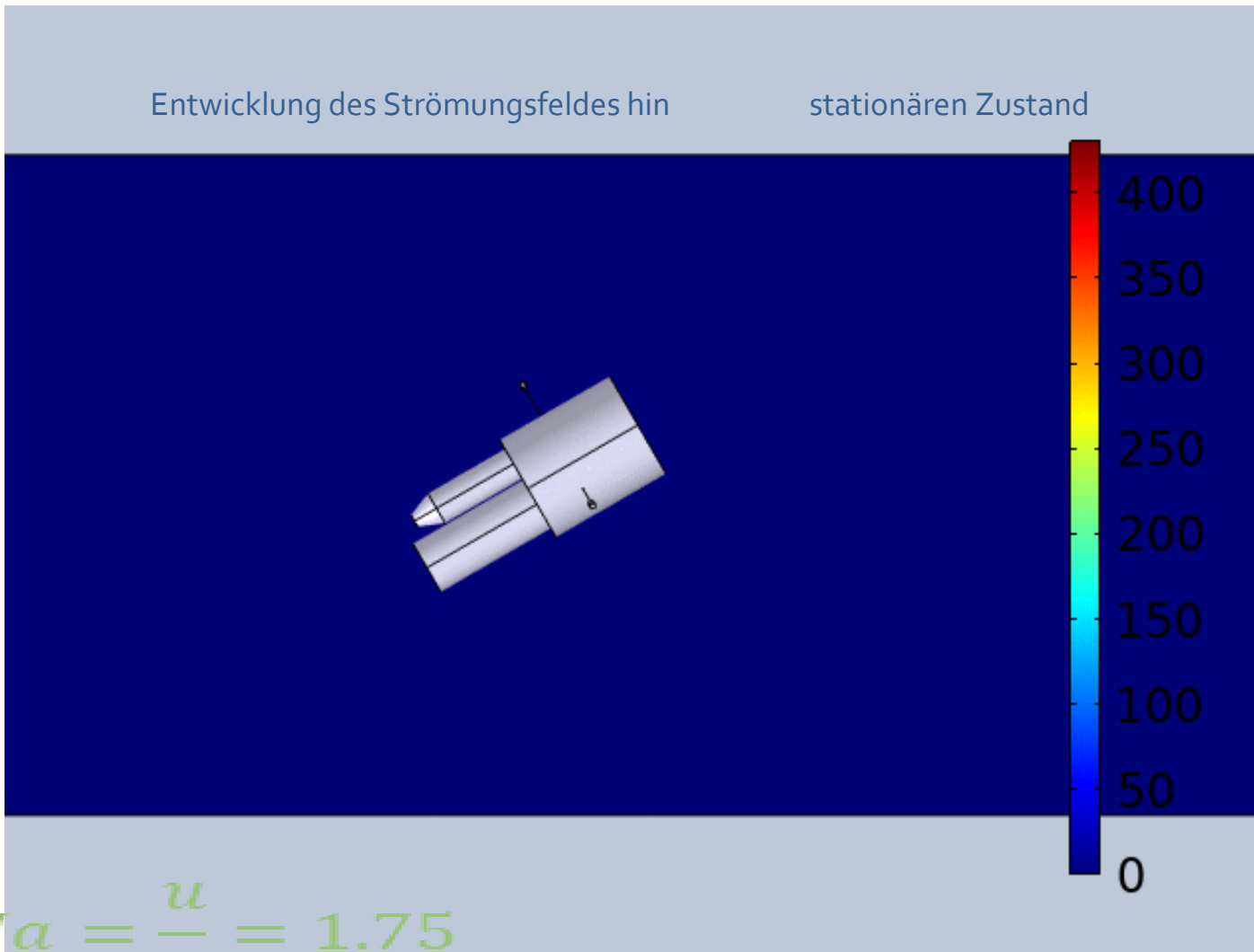
Generalized alpha methode





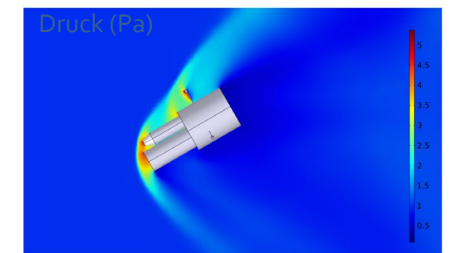
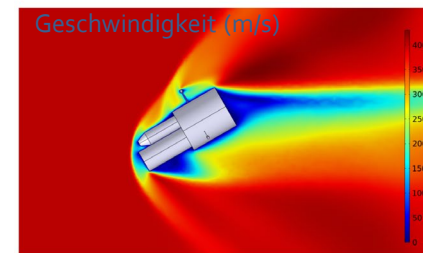
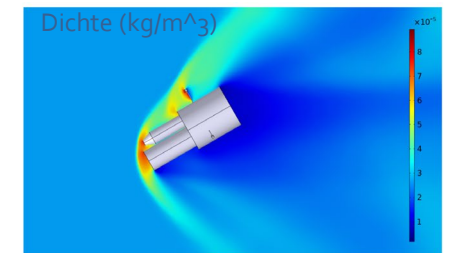
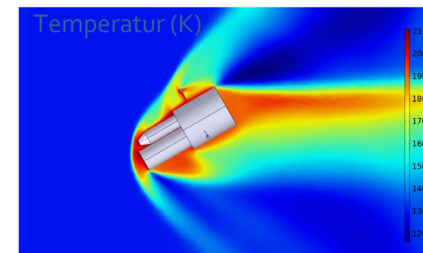
GEL Projekt

Simulation einer **supersonischen Strömung** um eine Höhenforschungsrakete und die **Sammeleffizienz von mesosphärischen Partikeln** auf Impaktorflächen

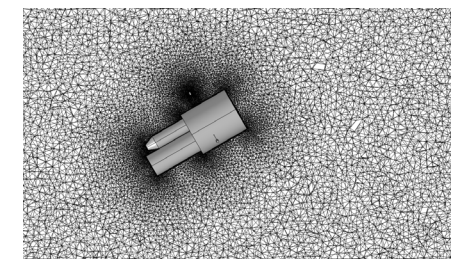


$$Ma = \frac{u}{c} = 1.75$$

$$Ma = \frac{u}{c} = 1.75$$
$$c_{85 \text{ km}} = \sqrt{\gamma R_s T} = 229 \frac{\text{m}}{\text{s}}$$



Stationäres Strömungsfeld

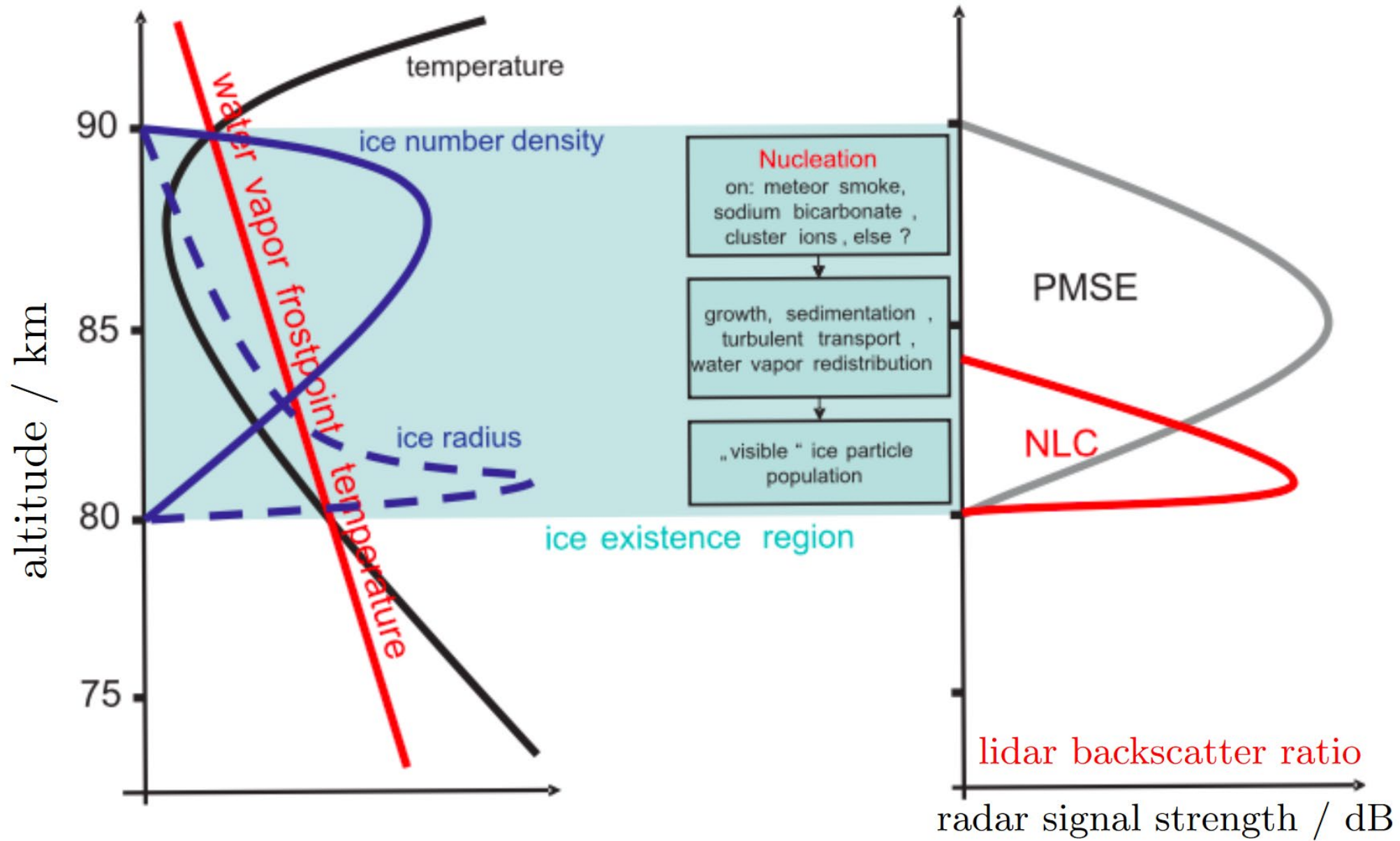


Berechnungsnetz

Meteoroid → Small (sub-km) rocky or metallic body in outer space.

Meteor → Light phenomenon ("shooting star" or "falling star"), visible passage of a frictionally heated and glowing body from outer space.

Meteorite → Solid piece or debris from outer space which has survived the passage through the atmosphere and has hit the surface → **Micrometeorite** if $D_p < 1$ mm.



| forces and their relationship R to the Stokes drag force | importance in reference to Stokes drag force |
|--|--|
| pressure gradient force: $R_p = \left \frac{\vec{F}_p}{\vec{F}_D} \right \sim \frac{d_p^2 \nabla p}{\vec{u}_r}$ | Neglectable for nanometre-sizes of d_p and small pressure gradients around the particle. |
| gravitational force: $R_{G,tot} = \left \frac{\vec{F}_g}{\vec{F}_D} \right \sim \frac{d_p^2}{\vec{u}_r}$ | Neglectable for nanometre-sized particles. |
| Saffman force: $R_L = \left \frac{\vec{F}_L}{\vec{F}_D} \right \sim d_p \sqrt{\frac{\vec{u}_r \times [\nabla \times \vec{u}_r]}{\vec{u}_r}}$ | Neglectable for nano size particles or small relative velocities. |
| added mass force: $R_{am} = \left \frac{\vec{F}_{am}}{\vec{F}_D} \right \sim d_p^2 \frac{d(\vec{u}_f - \vec{v}_p)}{dt}$ | Small for very small particles and for a small relative acceleration of the particle. |
| Brownian force: $R_{Brown} = \left \frac{\vec{F}_{Brown}}{\vec{F}_D} \right \sim \sqrt{\frac{1}{d_p \vec{u}_r^2}}$ | Indispensable for nanometre-sized particles. |

$$Ma = \frac{|v|}{c}, \quad c = \sqrt{\gamma R_s T},$$

$$c_{85 \text{ km}} = 229 \frac{\text{m}}{\text{s}}$$

$$v_{\min} = 300 \frac{\text{m}}{\text{s}}$$

$$v_{\max} = 400 \frac{\text{m}}{\text{s}}$$

$$Ma_{\min} = 1.31$$

$$Ma_{\max} = 1.75$$

$$Ma = \frac{|v|}{c}, \quad c = \sqrt{\gamma R_s T},$$

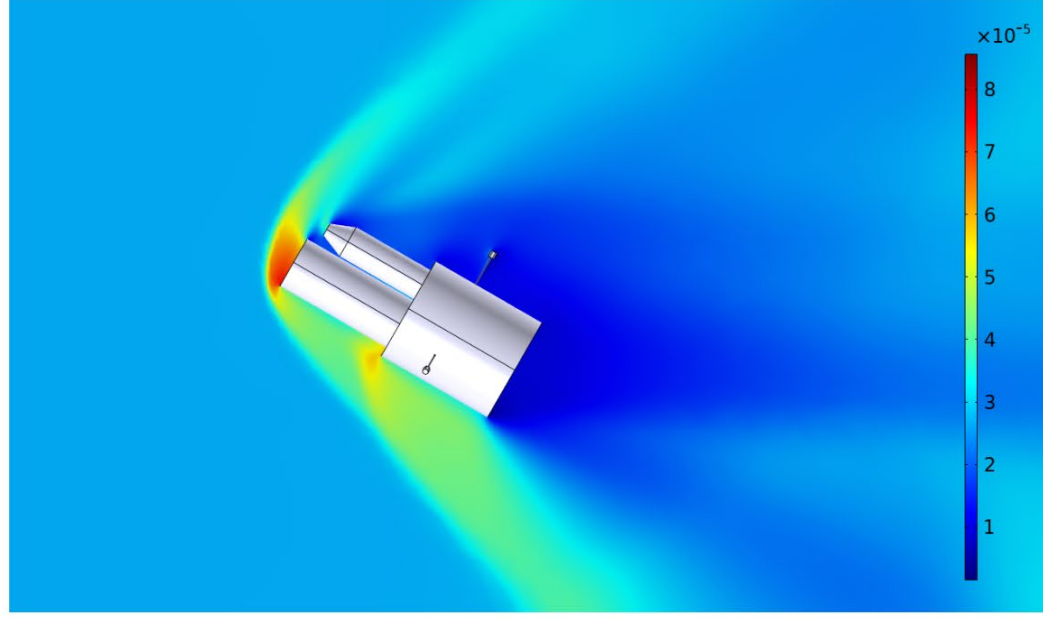
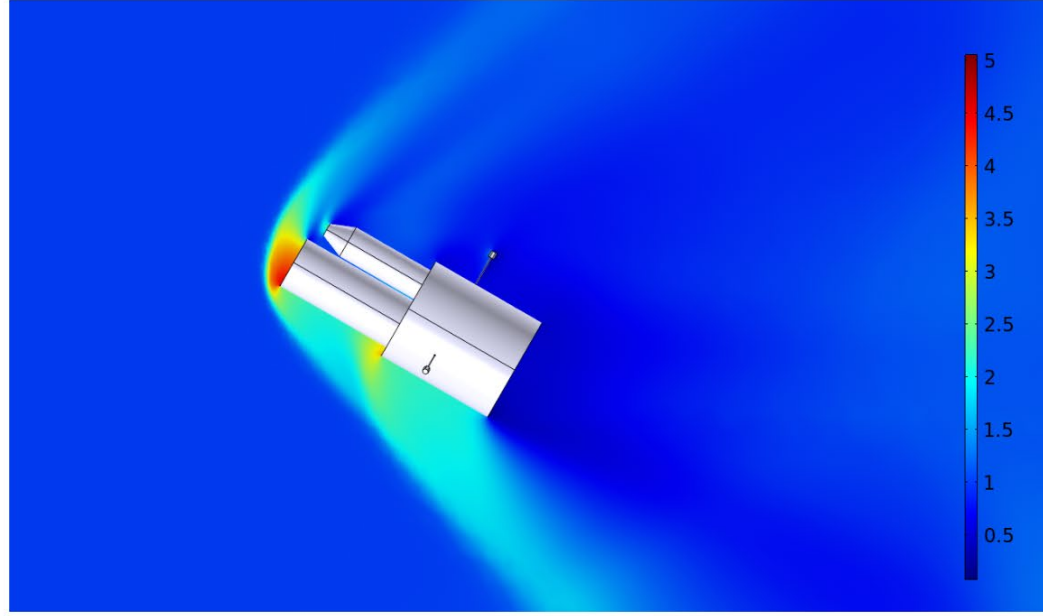
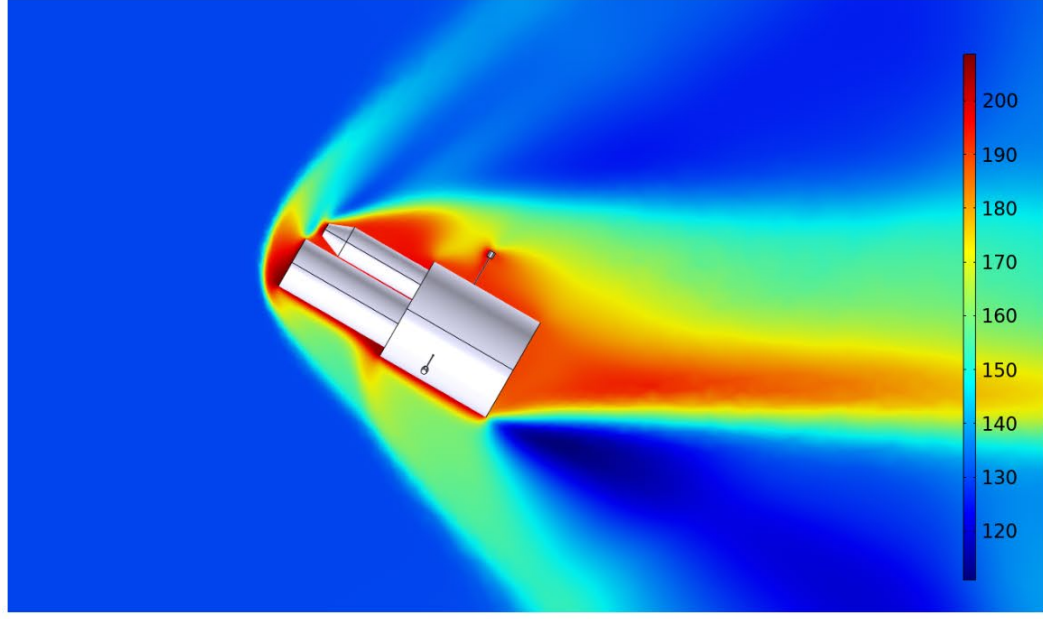
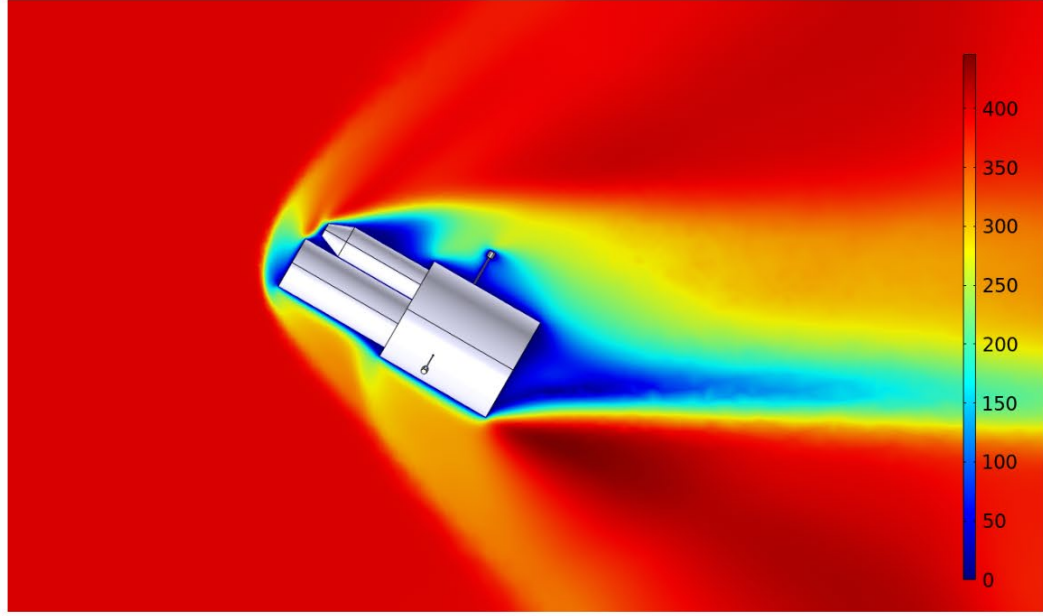
$$\underbrace{\frac{\partial \rho}{\partial t}}_{\text{temporal change of mass}} + \underbrace{\nabla \cdot (\rho \vec{u})}_{\text{change of mass flux}} = 0.$$

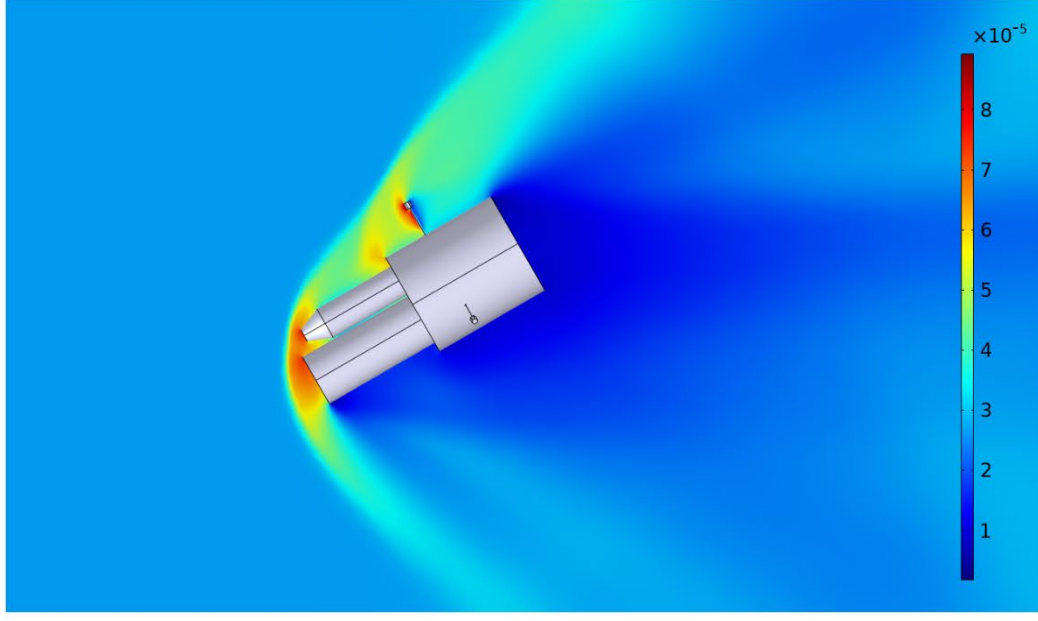
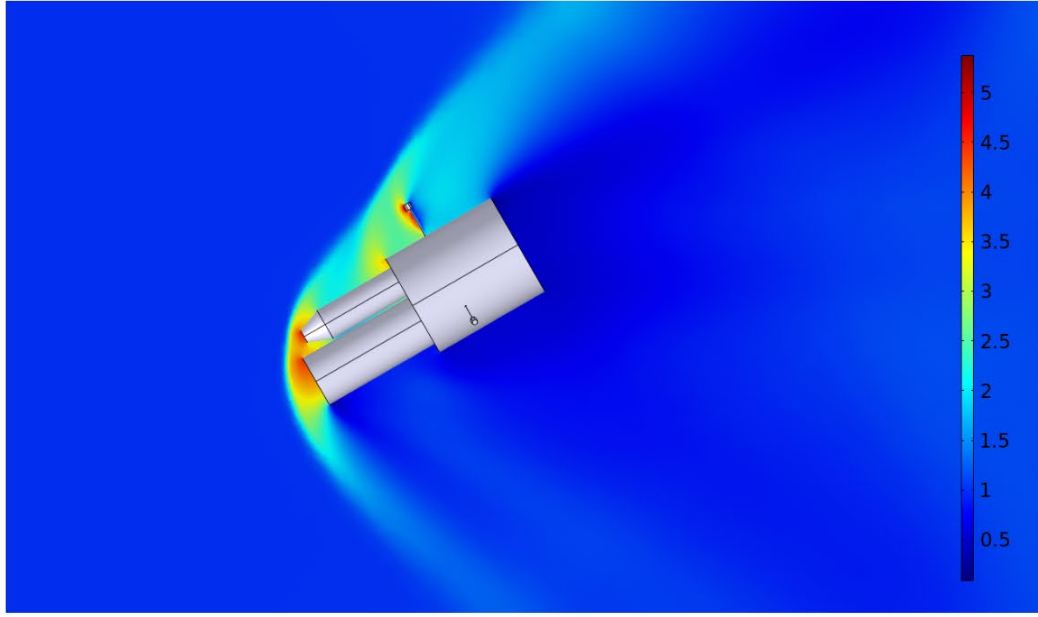
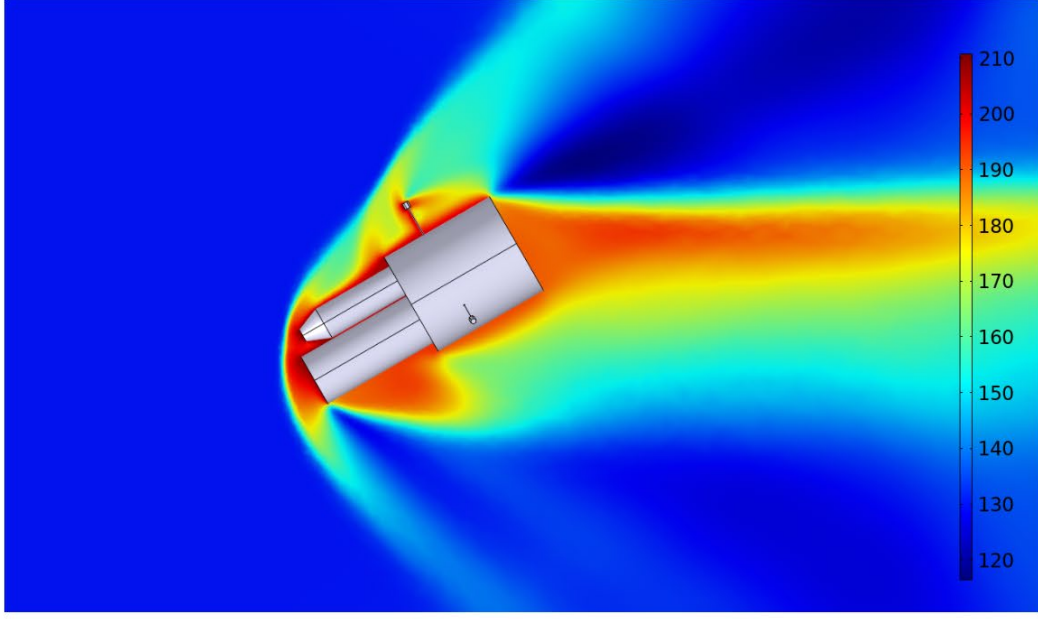
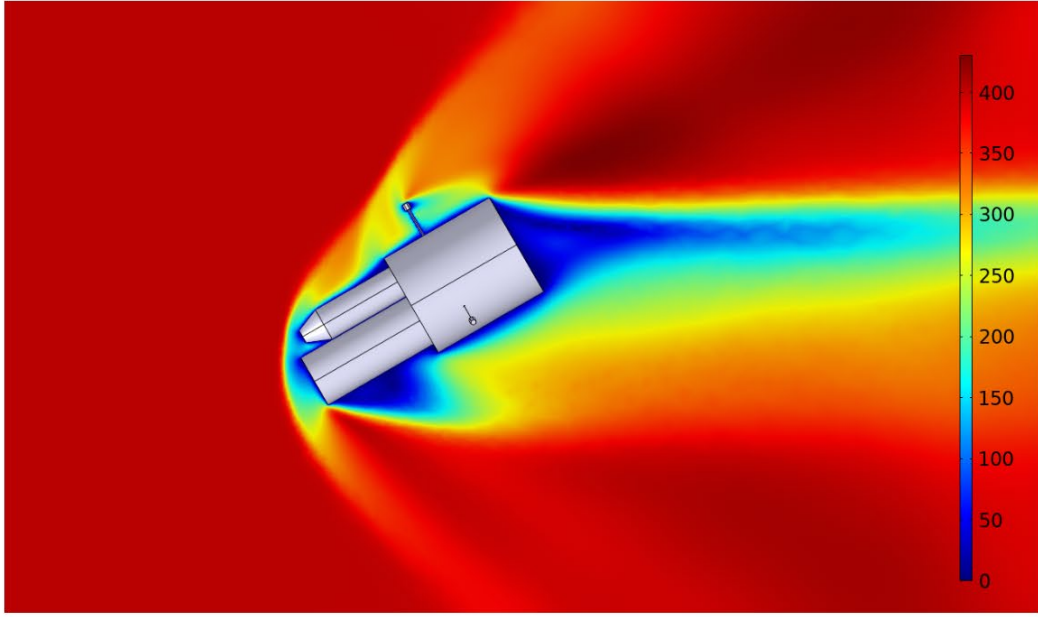
$$\underbrace{\rho \frac{\partial \vec{u}}{\partial t}}_{\text{temporal change of momentum}} + \underbrace{\rho(\vec{u} \cdot \nabla)\vec{u}}_{\text{change of momentum by advection}} = \underbrace{-\nabla p \mathbf{I}}_{\text{force from pressure gradient}} + \underbrace{\mu \Delta \vec{u}}_{\text{viscous shear surface force}} + \underbrace{\rho \vec{f}}_{\text{body force}}.$$

$$\underbrace{\frac{\partial}{\partial t} \left[\rho \left(e + \frac{u^2}{2} \right) \right]}_{\text{temporal change of total energy}} + \underbrace{\nabla \cdot \left[\rho \vec{u} \left(e + \frac{u^2}{2} \right) \right]}_{\text{net rate of flow of total energy}} = \underbrace{\nabla \cdot \vec{q}}_{\text{heat addition}} + \underbrace{\nabla \cdot (\sigma \vec{u})}_{\text{work due to pressure force}} + \underbrace{\rho(\vec{f} \cdot \vec{u})}_{\text{work due to body force}}.$$

$$e = c_v T,$$

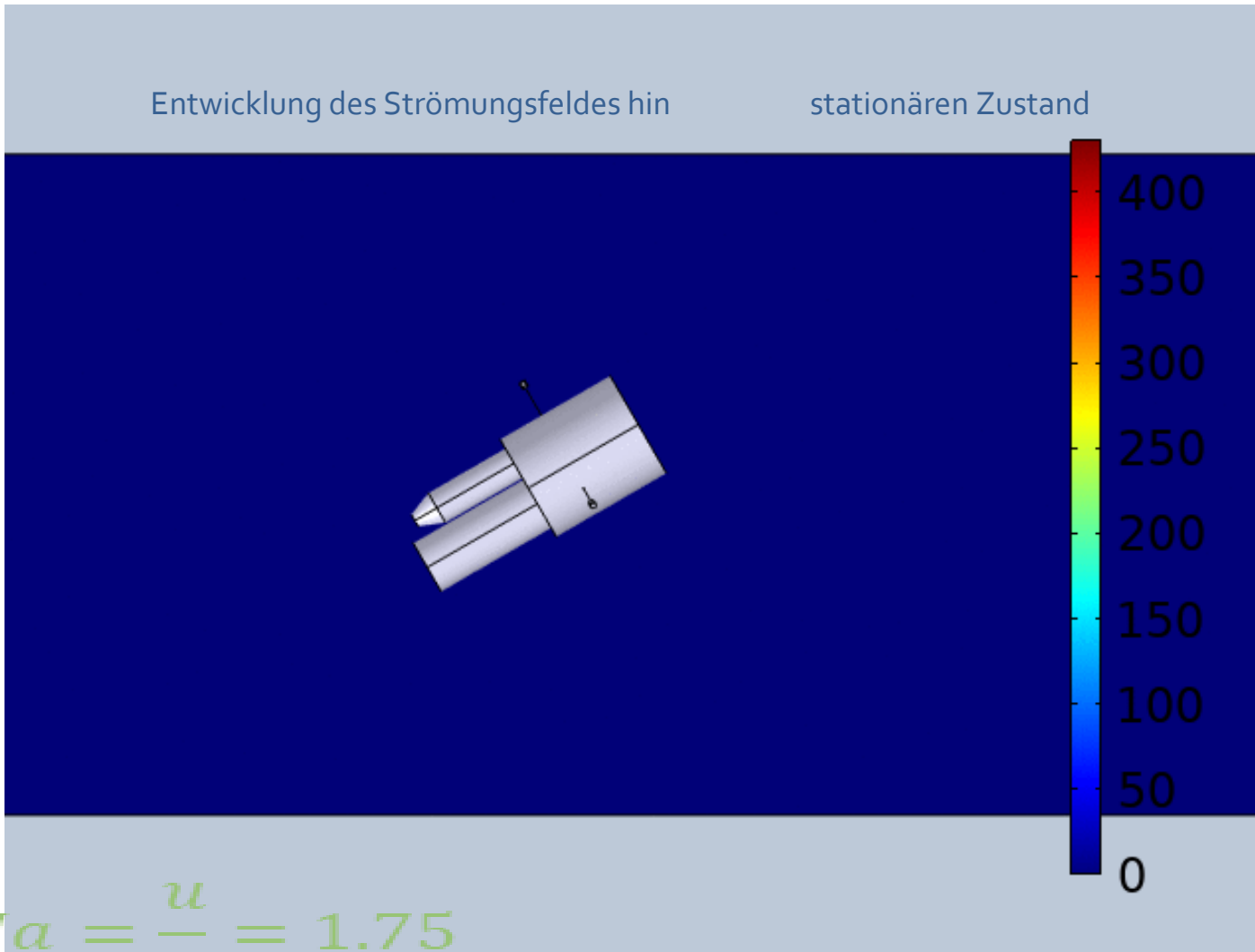
$$\rho = \frac{p}{R_s T},$$





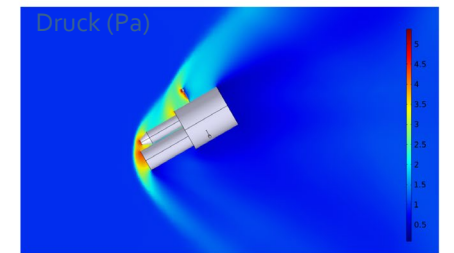
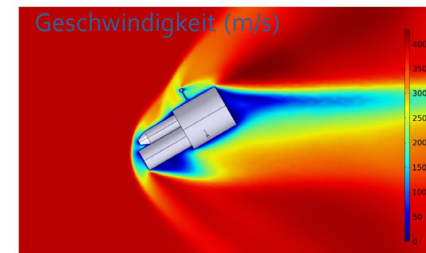
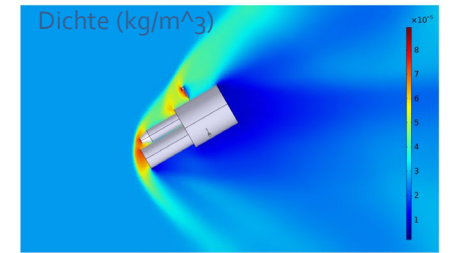
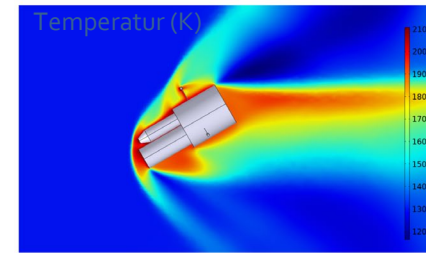
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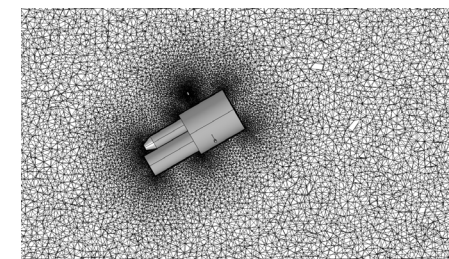


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Stationäres Strömungsfeld



Berechnungsnetz