Development of an evaporation boundary condition for DSMC method with application to meteoroid entry

F. Bariselli, S. Boccelli, A. Frezzotti, A. Hubin, T. Magin

Annual METRO meeting
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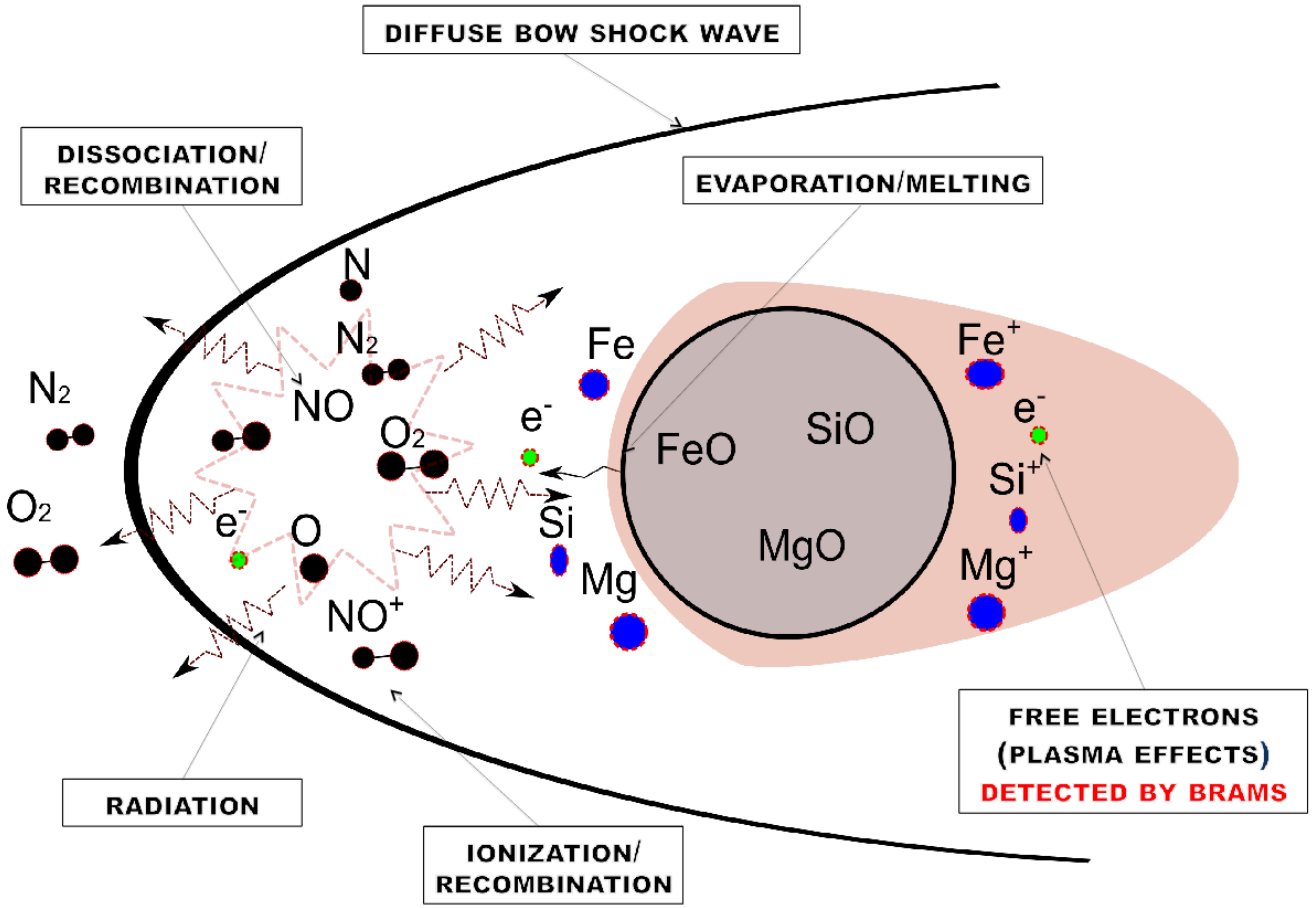
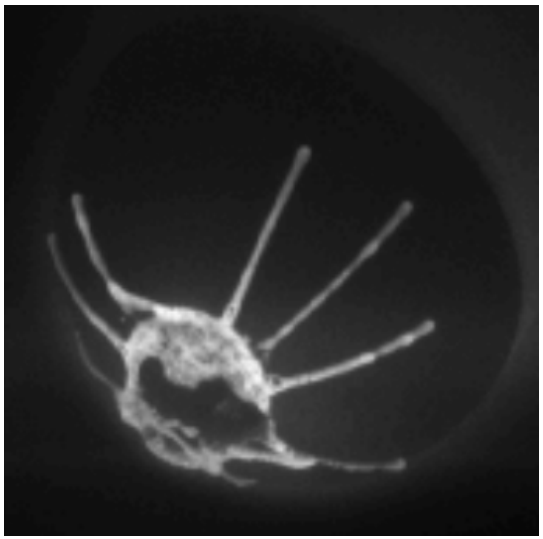
Physics of a meteoroid entering the atmosphere



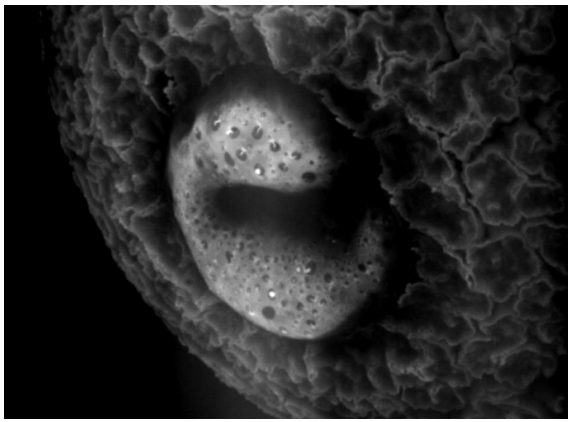
Coupled physico-chemical phenomena occurring during meteoroid ablation

- Velocity: **from 12 km/s to 72 km/s**
- Size: **from micro size grains to meters**

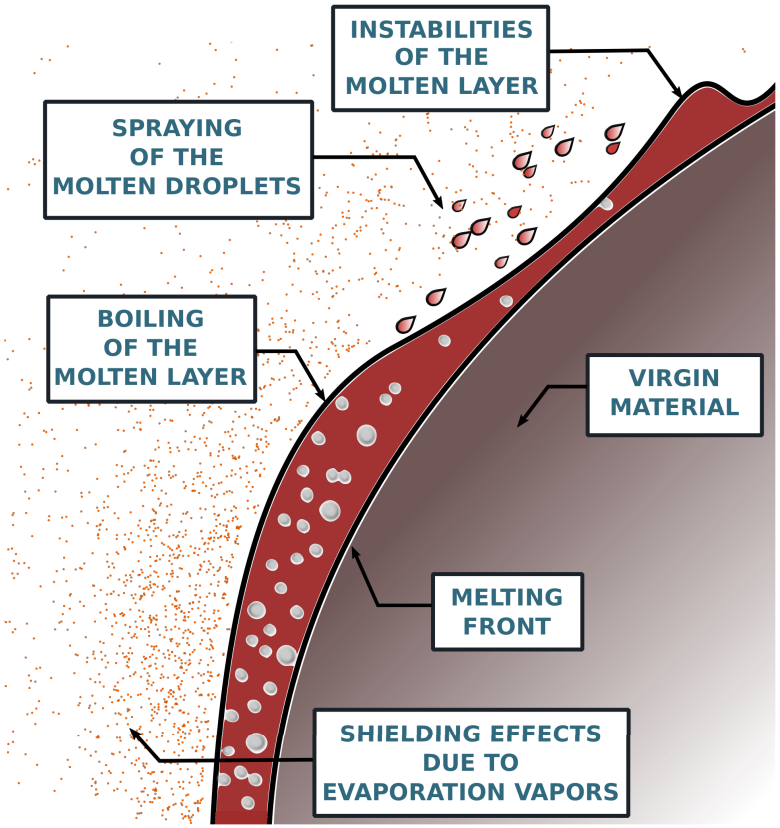
Focus on the gas-surface phenomena



VKI Plasmatron experiment: **basaltic sample**, 3 MW/m^2 heat flux at the stagnation point



Ordinary chondritic sample, 1 MW/m^2 heat flux at the stagnation point



Schematic of gas-surface interactions

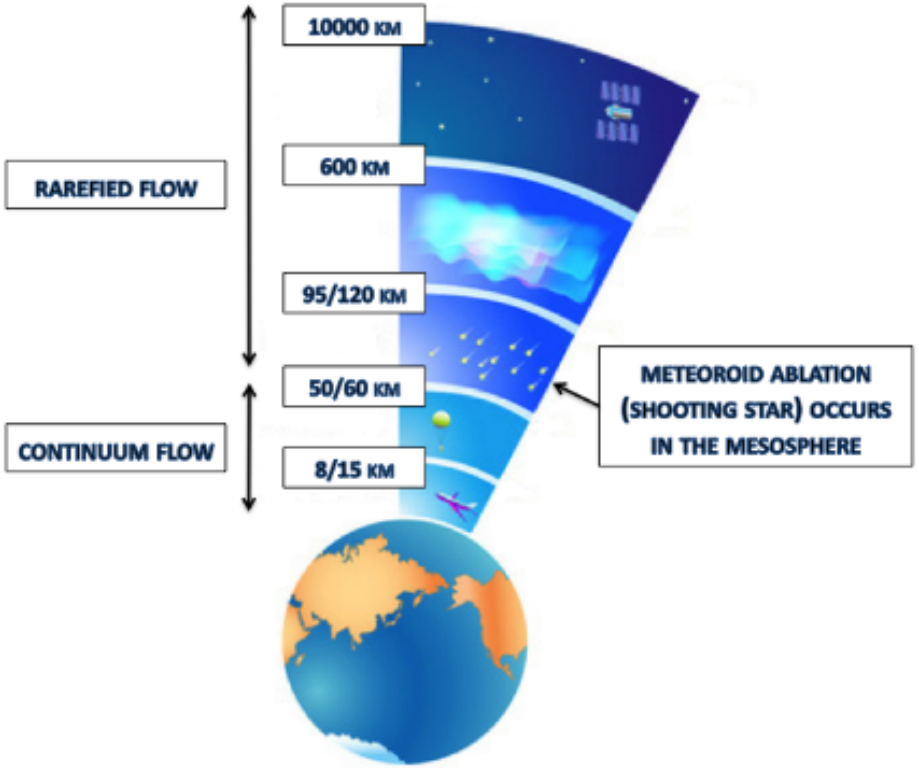
Objectives

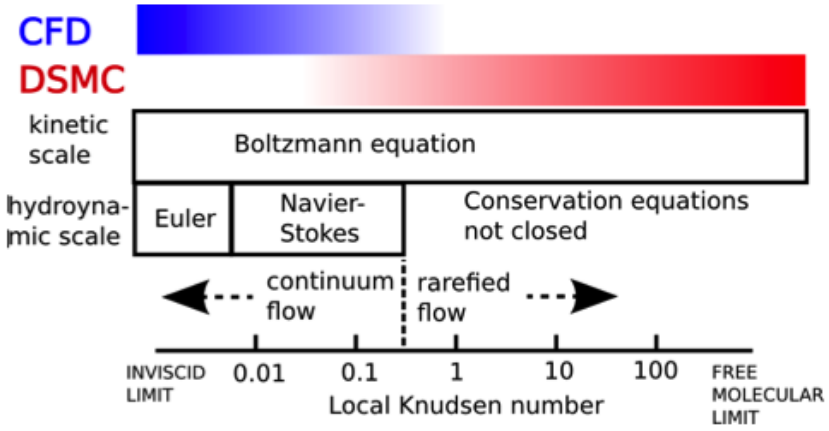
Goals

- Asses the importance in the competition among the different phenomena
- Develop an **evaporation boundary condition** capable of dealing with magma compositions (mixture of oxides)
- Couple the flow with the **material response**
- Introduce a method to compute **chemistry of ablated species**

1. Governing equations and numerical method
   - Boltzmann equation
   - Direct Simulation Monte Carlo method
   - SPARTA numerical tool
2. Ablative wall
   - Kinetic boundary conditions
   - Melt-vapor equilibrium
   - Extension to mixtures of oxides
3. Material response
   - Material code
   - Apparent heat capacity method
   - Interface flow-material
4. Trajectory code
5. Gas phase chemistry
   - Lagrangian solver
6. Conclusions and future work

Breakdown of the continuum regime

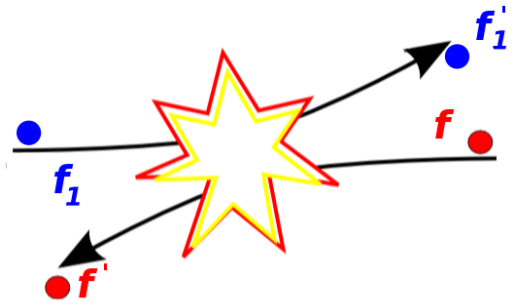




$$\textbf{Knudsen number} = \frac{\lambda}{D} = \frac{\text{mesoscopic scale}}{\text{macroscopic scale}}$$

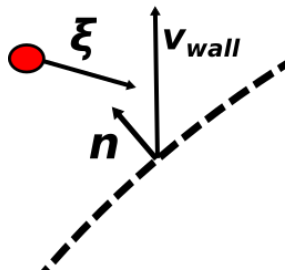
Boltzmann equation

$f(X, \xi, t)$ = **one-particle velocity distribution function**



$$\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial X} + F \cdot \frac{\partial f}{\partial \xi} = \overbrace{\int_{-\infty}^{\infty} \int_{0}^{4\pi} \left(f' f_1' - f f_1 \right) g \sigma \, d\omega \, d\xi_1}$$

From microscopic to macroscopic world:



$$\rho = \int_{-\infty}^{\infty} f(X, \xi, t) \, d\xi$$

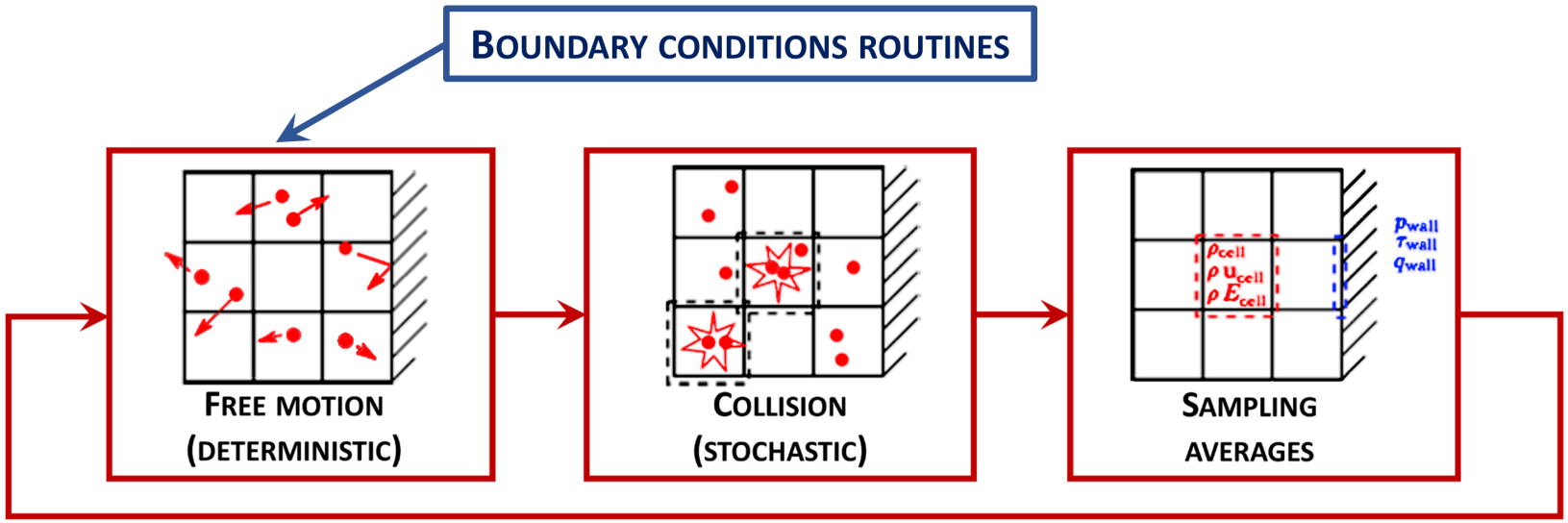
$$\rho V = \int_{-\infty}^{\infty} \xi \, f(X, \xi, t) \, d\xi$$

$$\rho e = \int_{-\infty}^{\infty} \frac{1}{2} \, \xi \cdot \xi \, f(X, \xi, t) \, d\xi$$

$$\varphi = \int_{-\infty}^{\infty} f(X, \xi, t) \, [\xi - v_w] \cdot n \, d\xi$$

$$q = \int_{-\infty}^{\infty} \frac{1}{2} \, \xi \cdot \xi \, f(X, \xi, t) \, [\xi - v_w] \cdot n \, d\xi$$

Direct Simulation Monte Carlo method

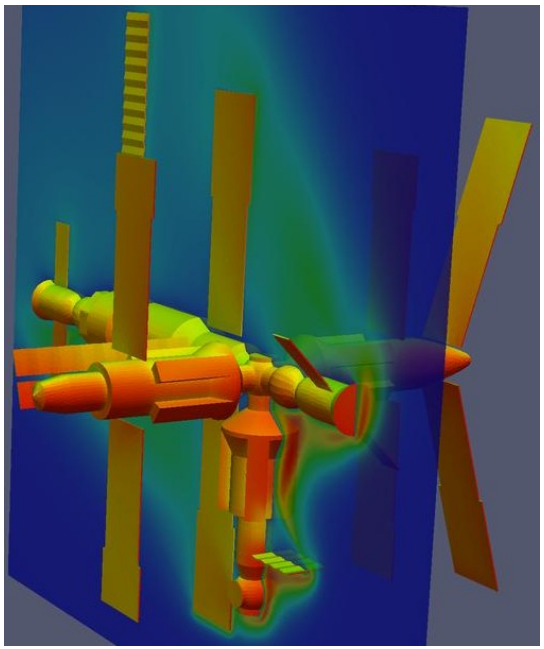


DSMC algorithm

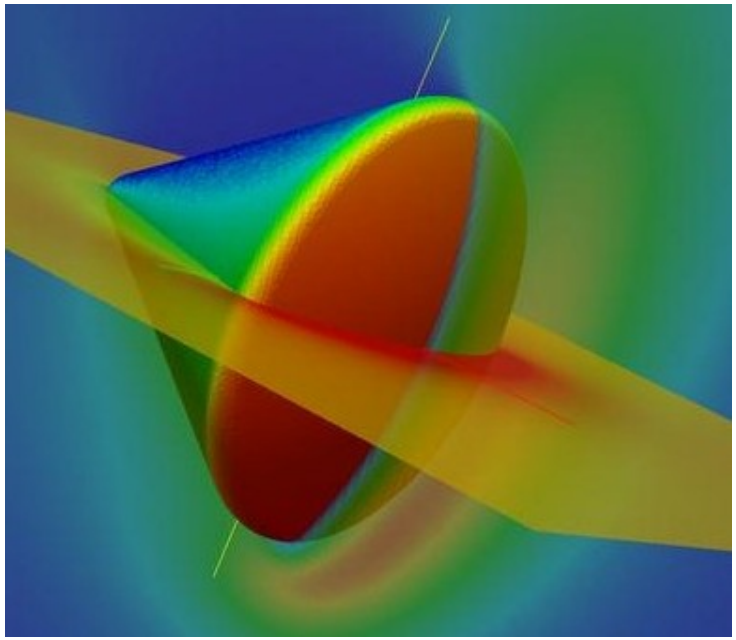
- Each simulated particle represents a large number of real particles
- Free motion decoupled from collisions (for $\Delta t < \nu_{coll}^{-1}$)
- Grid cells used to choose collisions partners and sample averages
- **DSMC is not Molecular Dynamics**

SPARTA numerical tool

- Developed by **Plimpton** and **Gallis** at Sandia National Labs
- **Open source** software (http://sparta.sandia.gov/)
- Object-oriented philosophy enables **extensions**
- **Parallel** implementation through domain decomposition



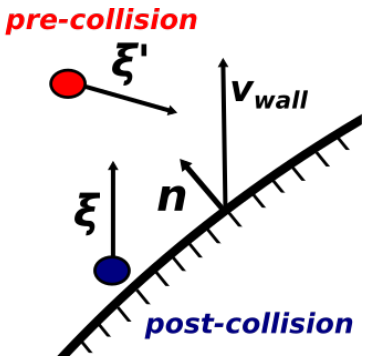
Flow around MIR space station



Apollo re-entering the atmosphere

Kinetic boundary conditions for Boltzmann equation

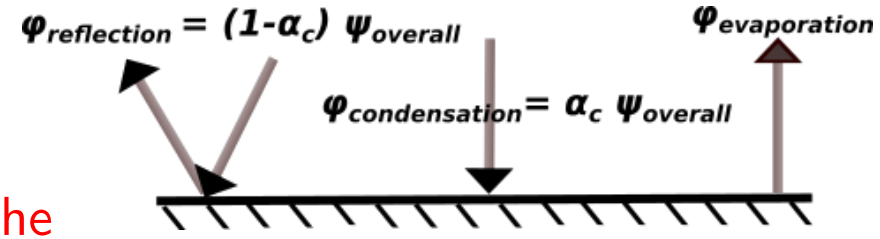
$$\overbrace{f(\boldsymbol{\xi})[\boldsymbol{\xi}-\boldsymbol{v_w}]\cdot\boldsymbol{n}}^{\text{flux emerging from the wall}} = \overbrace{g(\boldsymbol{\xi})[\boldsymbol{\xi}-\boldsymbol{v_w}]\cdot\boldsymbol{n}}^{\text{flux due to evaporation by the wall}} + \underbrace{\int_{[\boldsymbol{\xi'}-\boldsymbol{v_w}]\cdot\boldsymbol{n}<0} K_B(\boldsymbol{\xi'}\to\boldsymbol{\xi}) f(\boldsymbol{\xi'})[\boldsymbol{\xi'}-\boldsymbol{v_w}]\cdot\boldsymbol{n}\, d\boldsymbol{\xi'}}_{\text{flux due to reflection by the wall}} \qquad [\boldsymbol{\xi}-\boldsymbol{v_w}]\cdot\boldsymbol{n}>0$$



$$K_B(\boldsymbol{\xi'}\to\boldsymbol{\xi}) = (1-\alpha_c)\frac{[\boldsymbol{\xi}-\boldsymbol{v_w}]\cdot\boldsymbol{n}}{2\pi(RT_w)^2}\, exp\Big(-\frac{|\boldsymbol{\xi}-\boldsymbol{v_w}|^2}{2RT_w}\Big)$$

$$g(\boldsymbol{\xi}) = \frac{\alpha_e\rho_w^{eq}}{(2\pi RT_w)^{3/2}}\, exp\Big(-\frac{|\boldsymbol{\xi}-\boldsymbol{v_w}|^2}{2RT_w}\Big)$$

- α_e/α_c evaporation/condensation coefficients (usually $\alpha_e=\alpha_c=1$)
- ρ_w^{eq} equilibrium vapor density
- No need to assume equilibrium of the gas with the wall

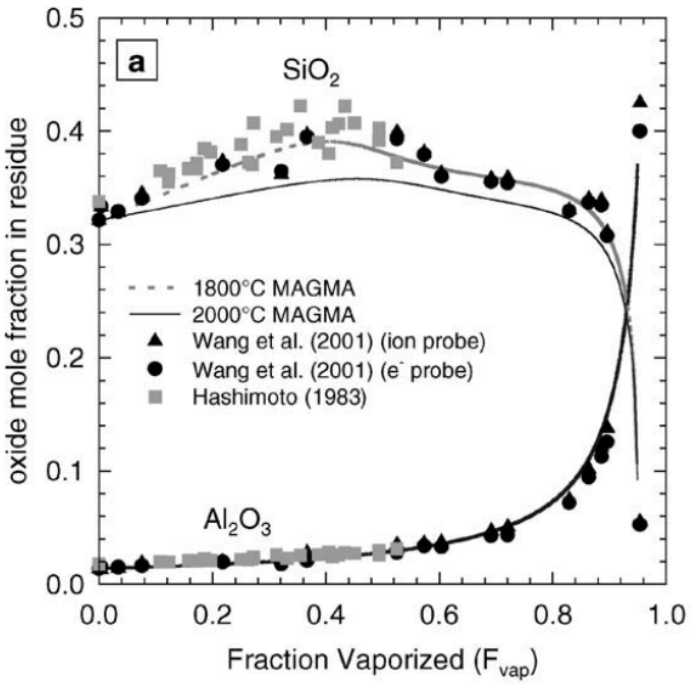


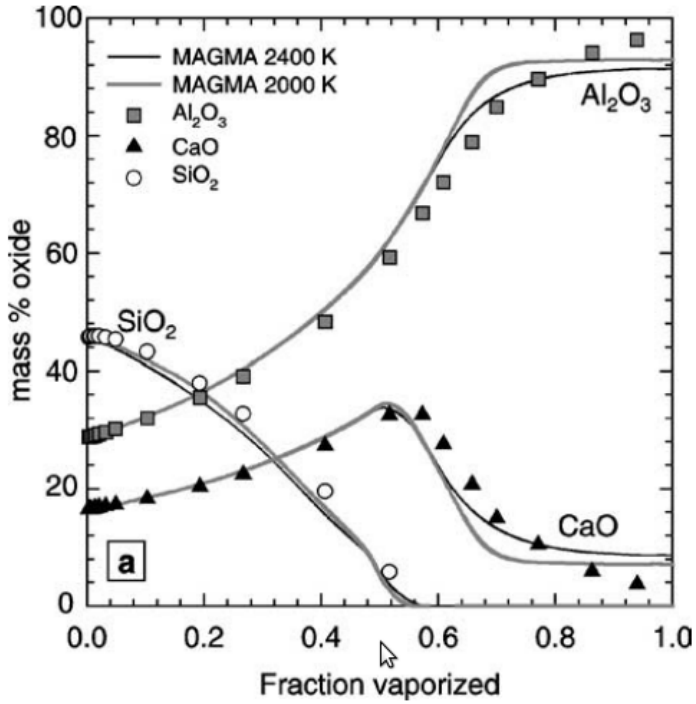
MAGMA chemical multi-phase equilibrium solver

How do we obtain the equilibrium properties?

$$\rho_{w_i}^{eq} = \rho_{w_i}^{eq}(\text{material composition}, T_w)$$

- Developed by **Fegley** and **Cameron**, 1987
- Mass balance, mass action algorithm
- Only stoichiometric reactions for change of phase
- Extensively validated vs. experimental data
- Already used to model vaporization in **silicate lavas** (under thermodynamic equilibrium assumption)





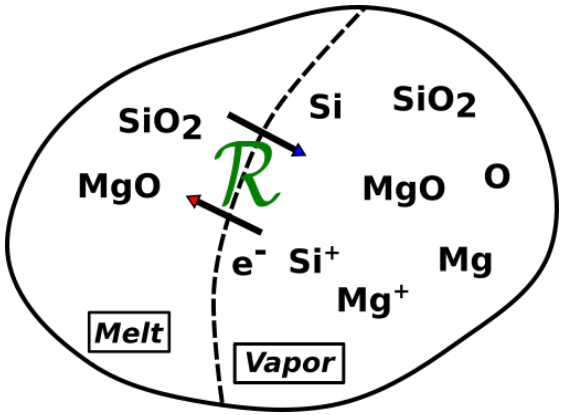
Extension to mixtures of oxides

How do we choose the coefficients?

$\alpha_{e_i}, \alpha_{c_i} \quad i \in \{\mathrm{O}, \mathrm{Si}, \mathrm{SiO_2}, \mathrm{Mg}, \mathrm{MgO}, \ldots\}$

- Hp. 0: $\boxed{\mathrm{M}_x\mathrm{O}_y\ (\mathrm{l}) \rightleftharpoons x\ \mathrm{M}\ (\mathrm{g}) + y\ \mathrm{O}\ (\mathrm{g})} \Rightarrow \alpha_{c_i} = 0 \ \ \forall\, i \neq \mathrm{M}, \mathrm{O}$
- Hp. 1: $\alpha_{c_\mathrm{M}} = \alpha_{e_\mathrm{M}} = \alpha_\mathrm{M} = \alpha$
- Hp. 2: $\alpha_{c_\mathrm{O}} = \alpha_{e_\mathrm{O}} = \alpha_\mathrm{O}$

$\Rightarrow$ **Thermodynamic equilibrium has to be retrieved by kinetic approach**



$$\varphi_i^{eq} = \varphi_i^{eq}(\alpha_i, \rho_{w_i}^{eq}, T_w)$$

$$\begin{cases} \varphi_{e_\mathrm{M}}^{eq} = \varphi_{c_\mathrm{M}}^{eq} \ \ \forall\ \mathrm{M} \\ \varphi_{e_\mathrm{O}}^{eq} = \varphi_{c_\mathrm{O}}^{eq} \ \ \Rightarrow \ \ \sum_{k \in R} \varphi_{e_{\mathrm{O}_k}}^{eq} = \varphi_{c_\mathrm{O}}^{eq} \\ y_k \varphi_{e_{\mathrm{M}_k}}^{eq} = x_k \varphi_{e_{\mathrm{O}_k}}^{eq} \ \ \forall\ k \in R \end{cases}$$

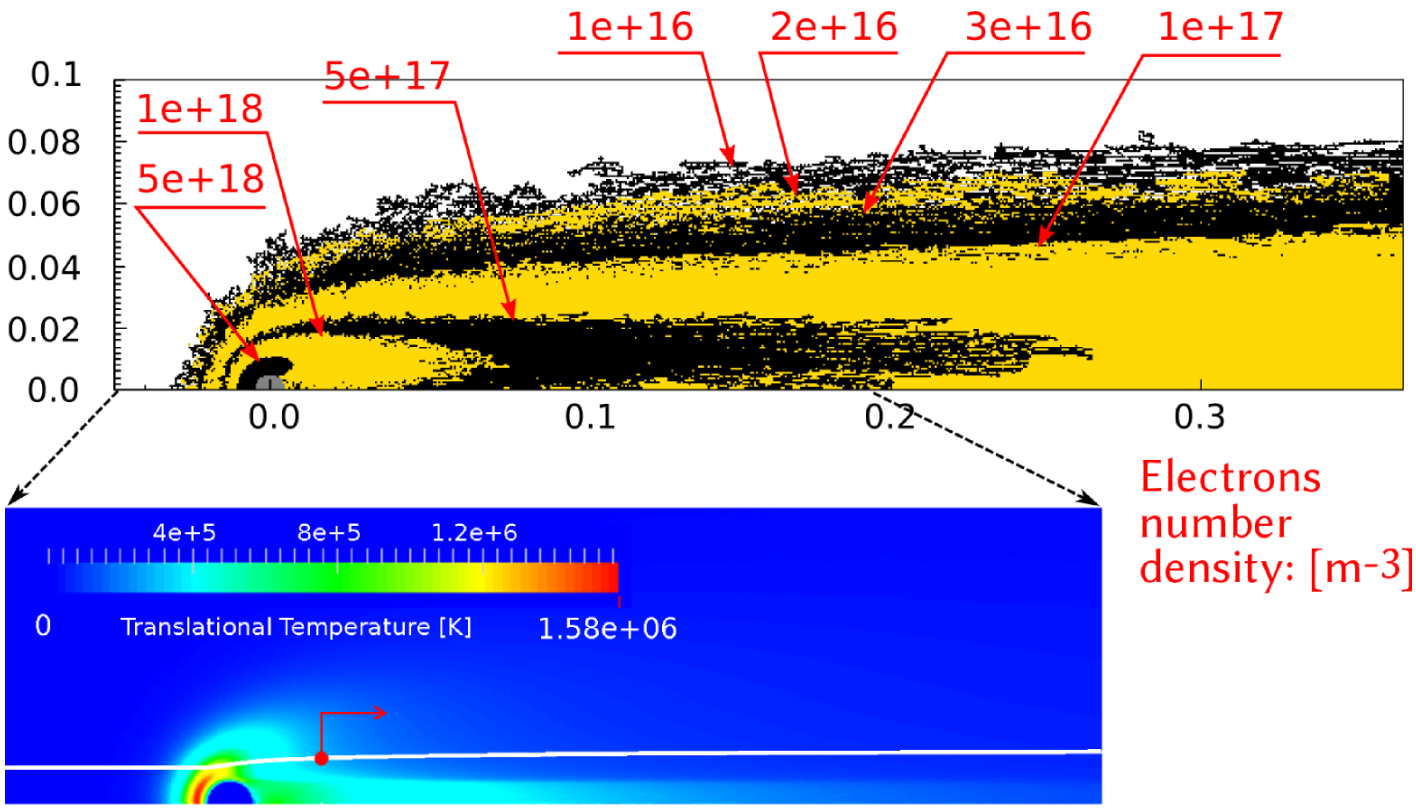
Electron concentration around a non-ablating meteoroid

- Kn = 0.1
- D = 1 cm
- H = 80 km
- V_∞ = 72 km/s

NON-ABLATING METEOROID

$10^{11} \div 10^{20}$ m^{-3} typical e^- density for meteors

Ambipolar diffusion assumption

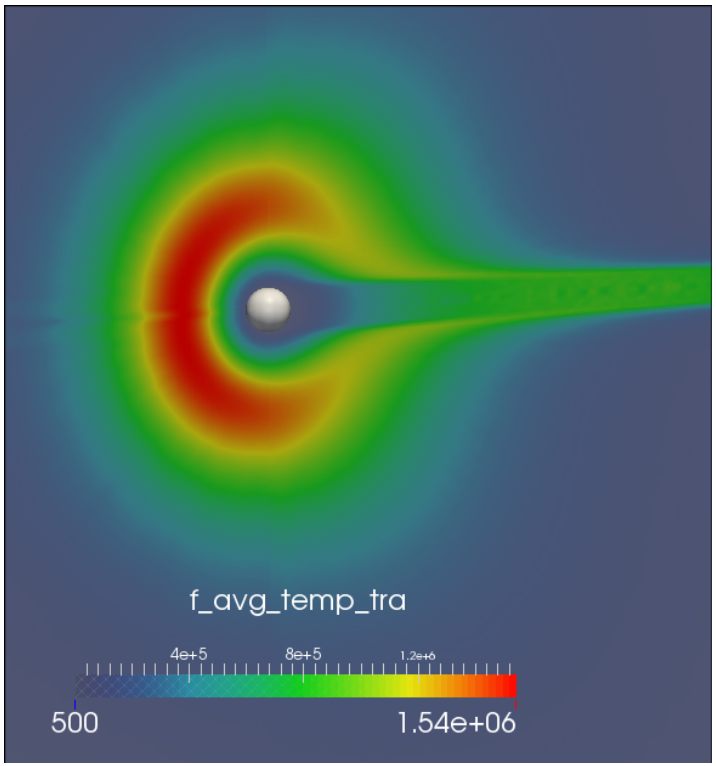


Gas phase chemistry frozen above 90 km $\Rightarrow$ electrons from metal species

Ablating meteoroid at 95 km altitude

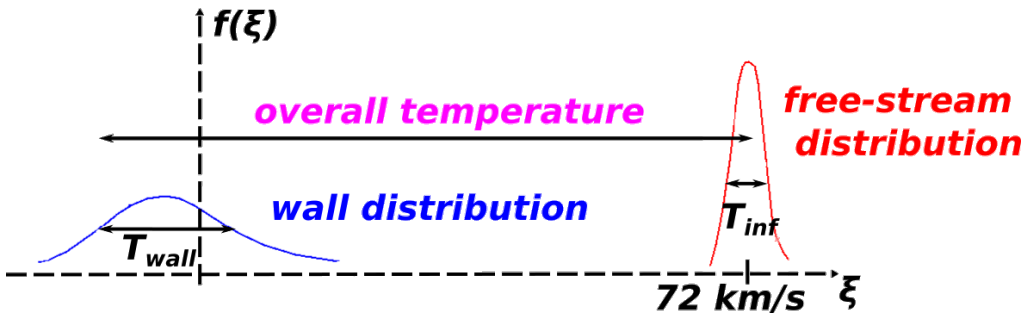
Pure magnesium:
$T_{wall} = 925$ K (**melting temperature**)
$v_{wall} = 0$ m/s
$\alpha_c = \alpha_e = 1$

- D = 1 cm
- H = 95 km
- $V_\infty = 72$ km/s



Translational temperature

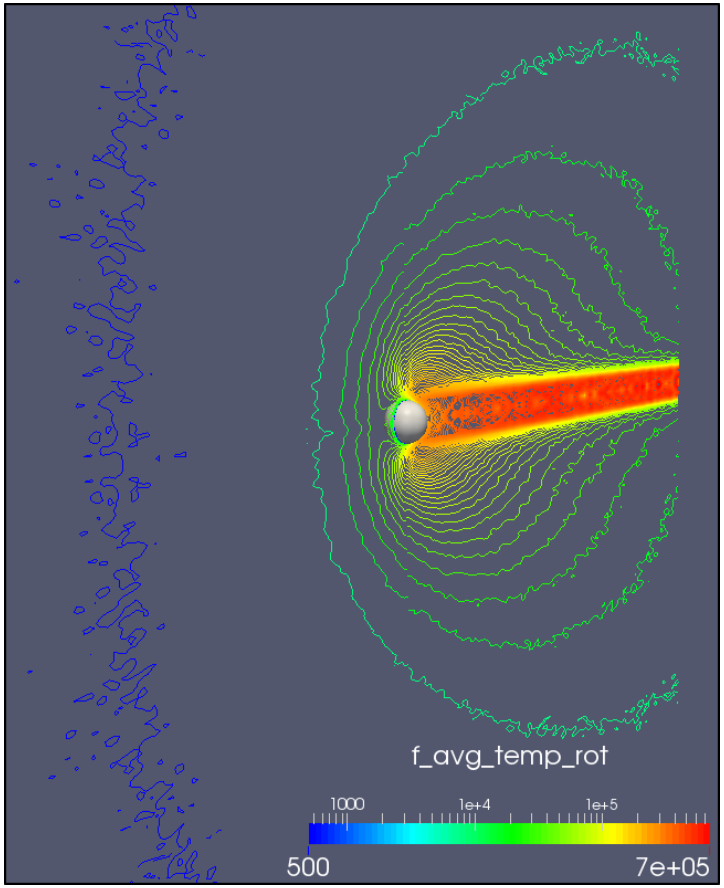
Cooling effect of evaporation at the wall
Adiabatic T $\approx$ 2.5M K >> T_{wall}
Geometric temperature: particles not characterized by this temperature in the thermal sense



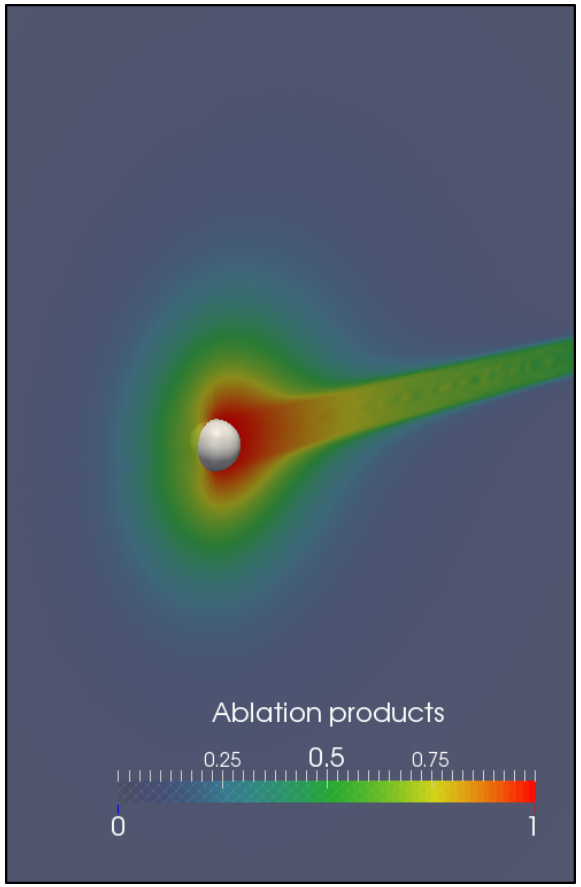
Ablating meteoroid at 95 km altitude

Delay in the excitation of the internal dofs

Strong shielding effects of Mg vapor



Rotational temperature



Ablation products molar fraction

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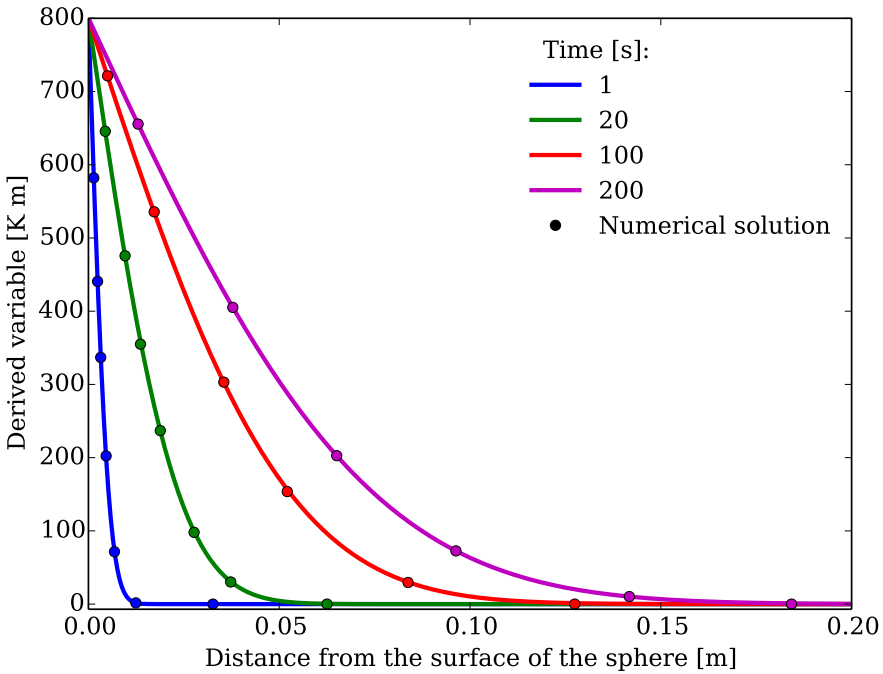
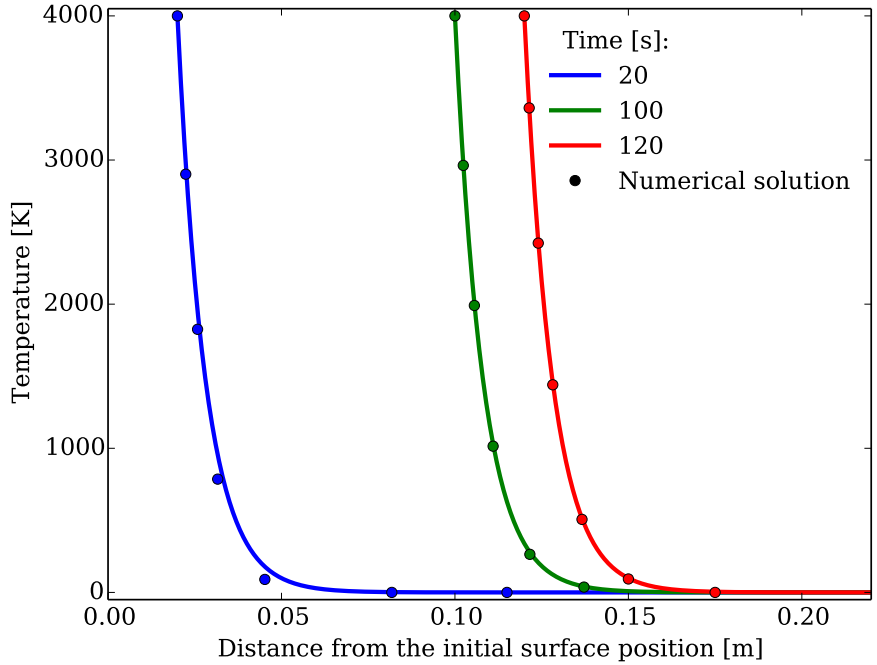
Material response

- **Randomly and rapidly rotating sphere**: $\frac{\partial T}{\partial t} = \frac{k}{\rho c_p}\frac{\partial^2 T}{\partial r^2} + \frac{2k}{\rho c_p}\frac{1}{r}\frac{\partial T}{\partial r}$
- Ablating wall: moving mesh (fixed reference frame)
- **Re-mapping procedure** at each time step
- Finite differences, explicit time integration

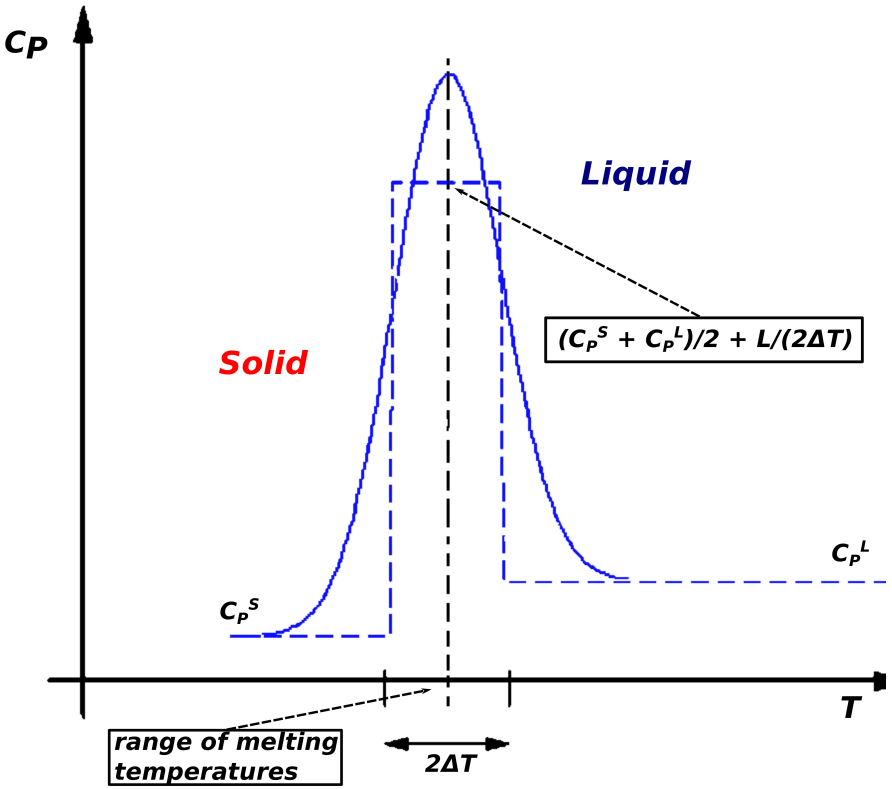


Verification of the **spherical coordinates**: unsteady solution

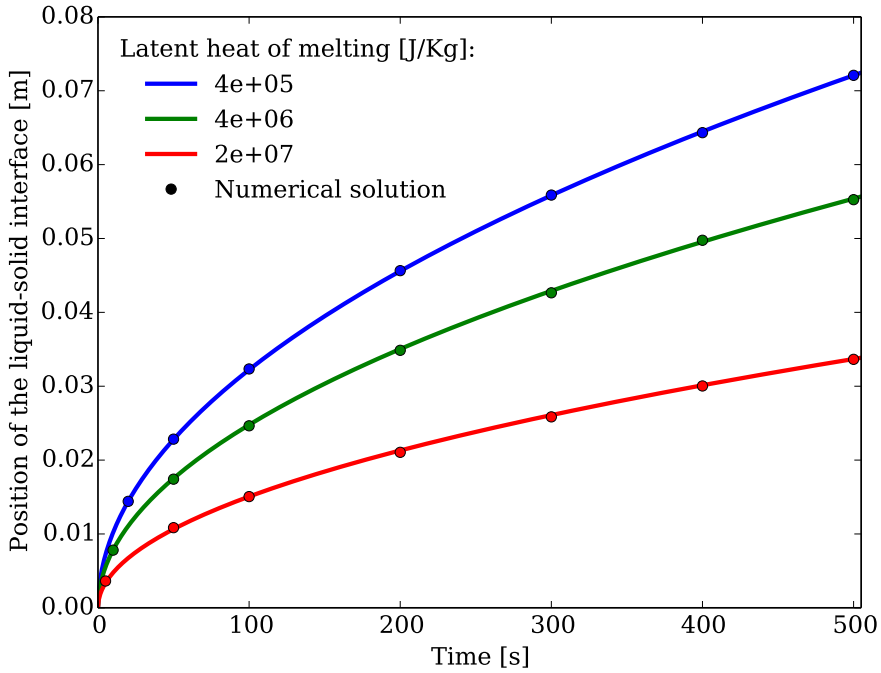


Verification of the **moving wall (re-mapping)**: steady solution

Tracking of the melting front



Heat capacity

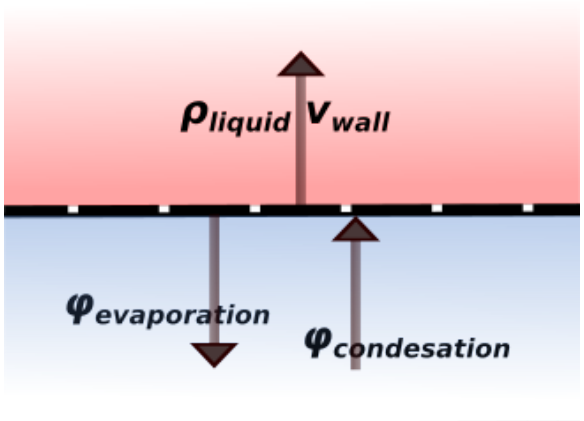


Verification of the apparent heat capacity method:

position of the melting front

- **Apparent heat capacity method**
- No need to deform the mesh to track the solid-liquid interface
- Position of the melting front obtained a posteriori

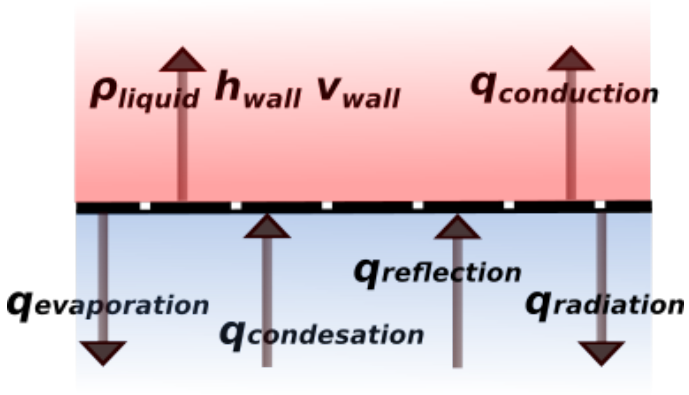
Interface flow-material



Surface mass balance

- $\varphi_e - \varphi_c = \rho_w v_w$
- φ_e computed theoretically
- φ_c directly from DSMC simulation
- No contribution of reflection (no net flux)

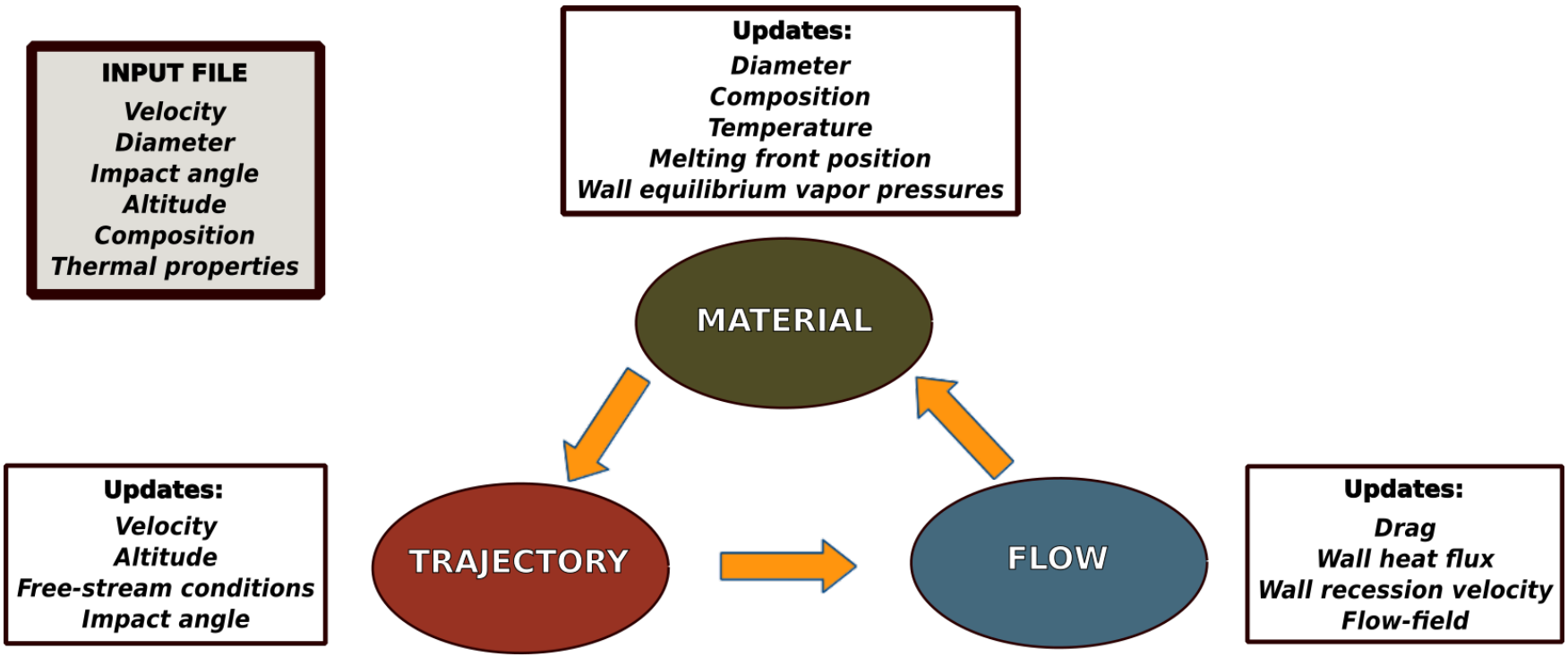
- $q_c + q_r - q_e + \epsilon\sigma T_\infty^4 = \rho_w h_w v_w + k \left.\frac{\partial T}{\partial r}\right|_w + \epsilon\sigma T_w^4$
- φ_e computed theoretically
- q_c, q_r directly from DSMC simulation



Surface energy balance

Trajectory code

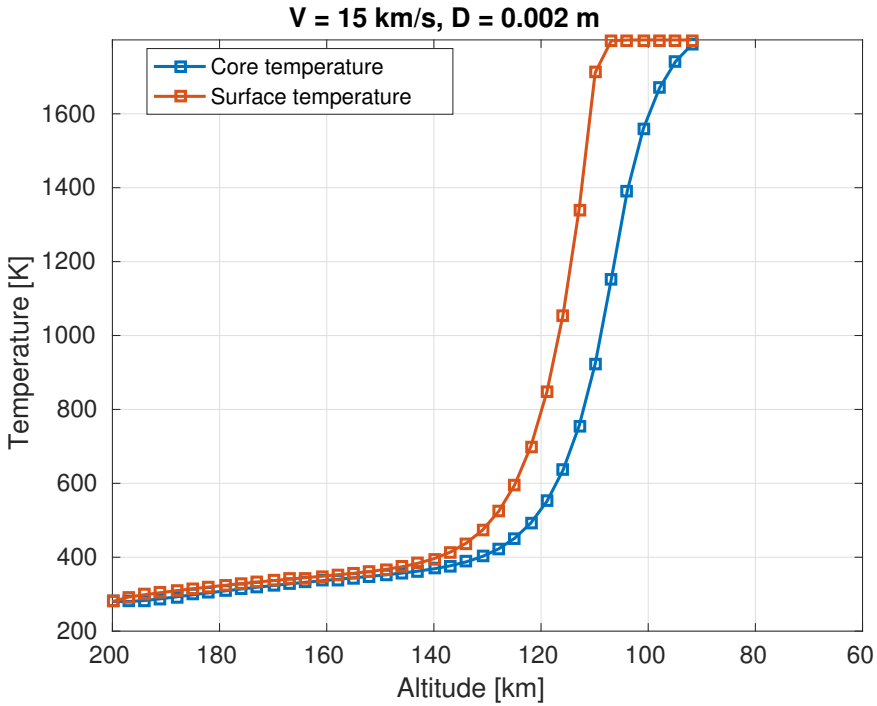
- Python implementation (cython to improve performances)
- Interface with MAGMA for wall equilibrium properties
- Interface with NASA atmospheric model for free-stream properties
- Sub time stepping for material response
- **Flow update resolution can be fixed through input file**

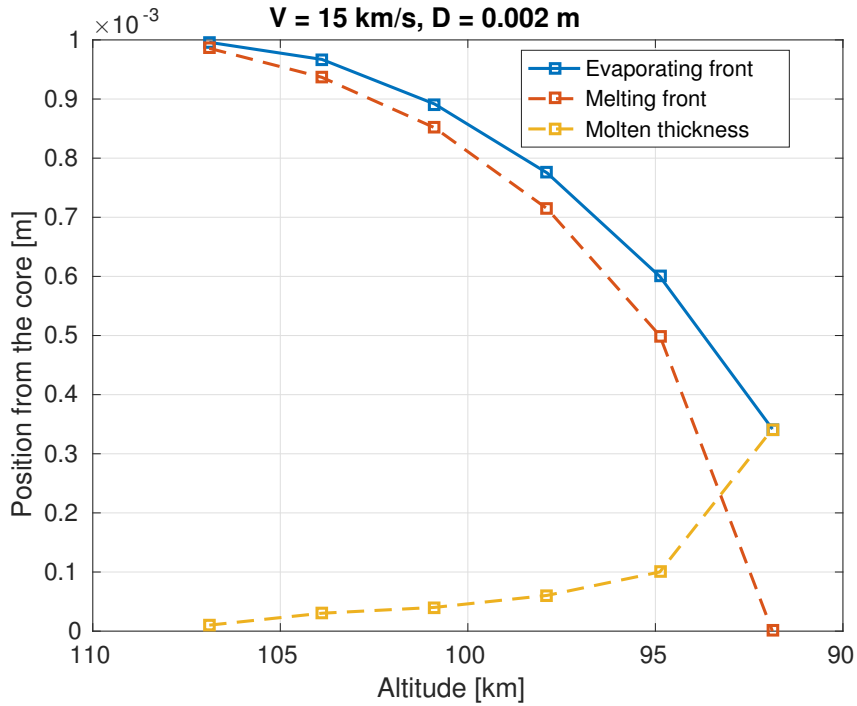


Trajectory-material response coupling

No DSMC coupling: evaporation into vacuum (**Knudsen-Langmuir**)

$$q_{flow} = \frac{\Lambda \rho_\infty(H) V_\infty^3}{8}$$



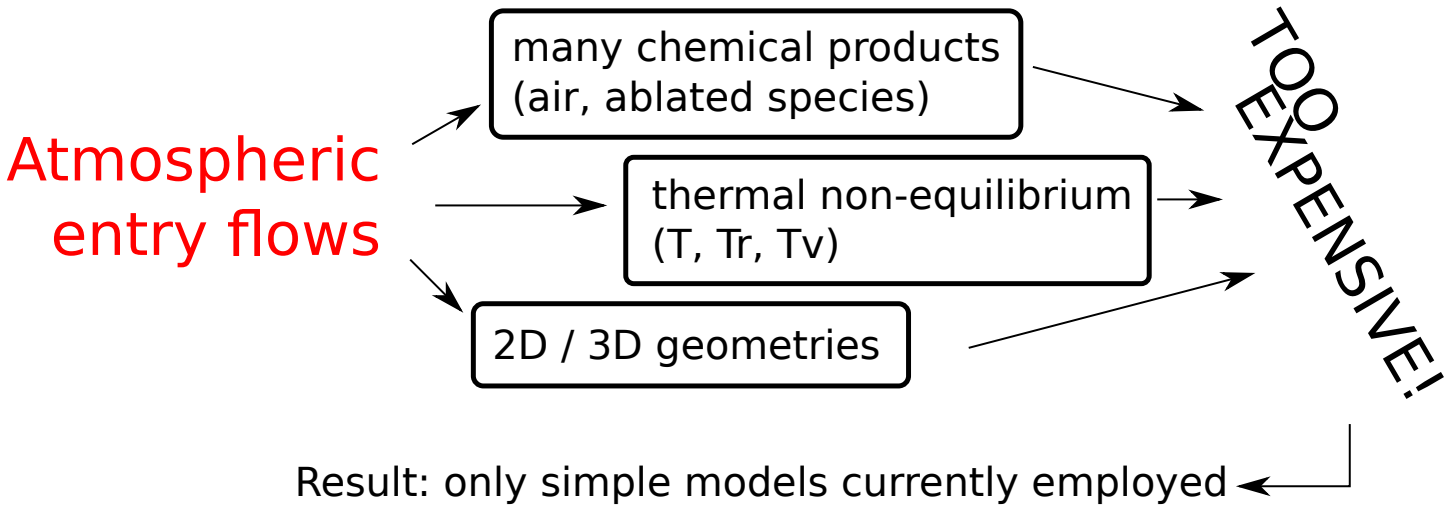


- D = 2 mm
- V_∞ = 15 km/s

Lagrangian solver

LARSEN

LAgrangian
Reactor for
Str**E**ams in
Nonequilibrium



Result: only simple models currently employed

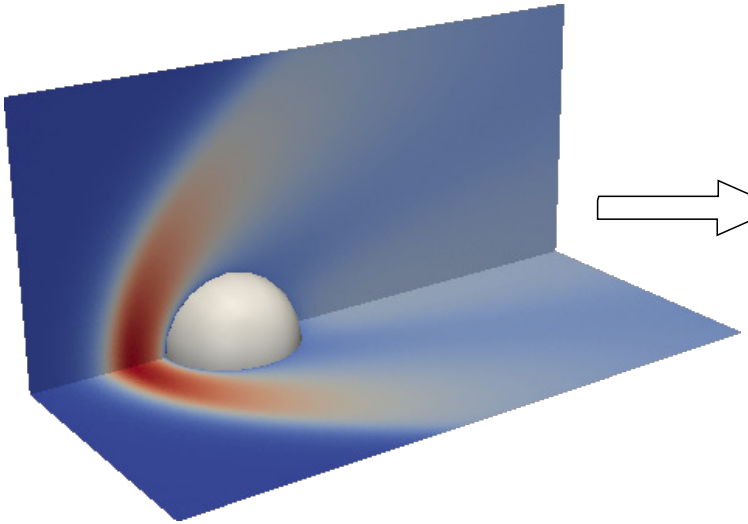
HOWEVER...

METEOROID TRAIL: detailled ionization mechanisms required...

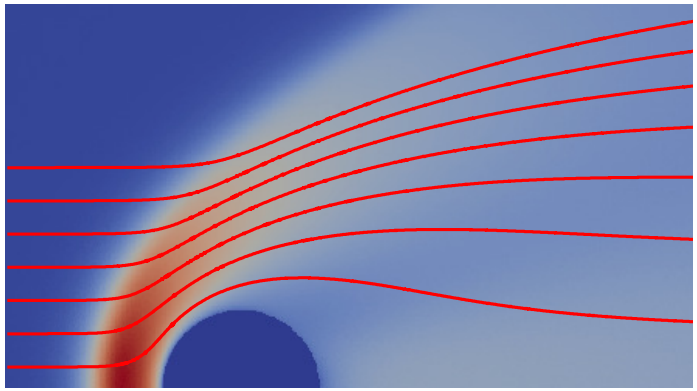
IDEA: introduce chemistry a posteriori!

Chemistry of ablated species computed *a posteriori*

1) Simple simulation



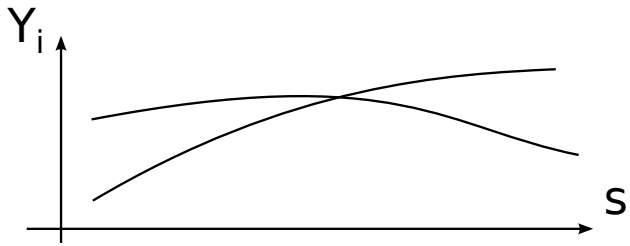
2) Extract streamlines



u(s) ρ(s) + ICs

3) Lagrangian solver

4) Refined results



Velocity and density fields from baseline simulation assumed good enough

LARSEN formulation

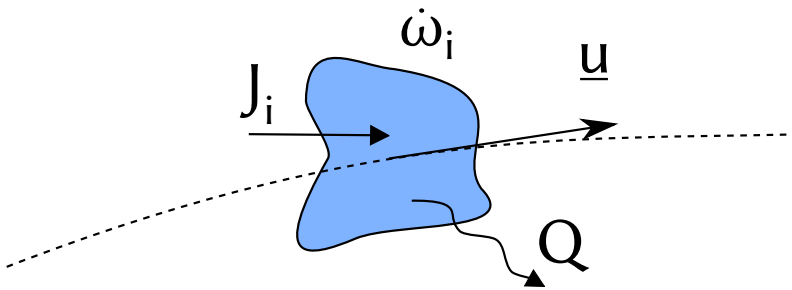
From baseline simulation: u, ρ are given

We still need:

$$\text{Species mass eq.} \quad \rightarrow \quad \partial_s y_i = \frac{\dot{\omega}_i - \nabla \cdot \boldsymbol{J}_i}{\rho u}$$

$$\text{Total enthalpy eq.} \quad \rightarrow \quad \partial_s H = \mathcal{Q}_{ext}$$

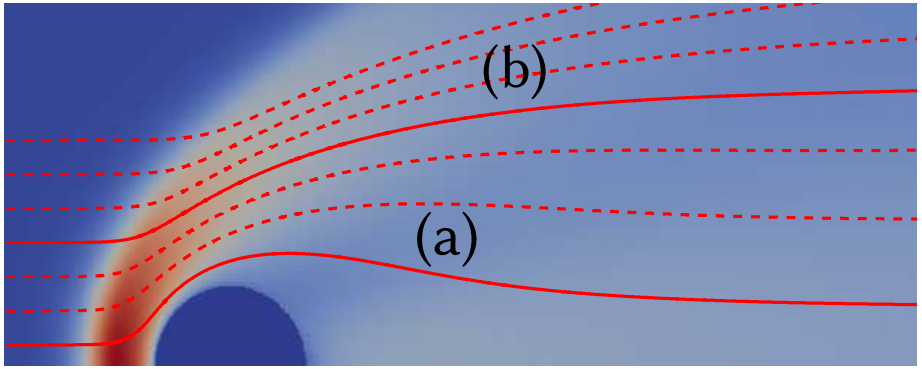
$$\text{Species internal energy} \quad \rightarrow \quad \partial_s e_i^{in} = \frac{\nabla \cdot \boldsymbol{D}_i^{in} + \Omega_i^{in} - h_i^{in}\dot{\omega}_i}{\rho y_i u}$$

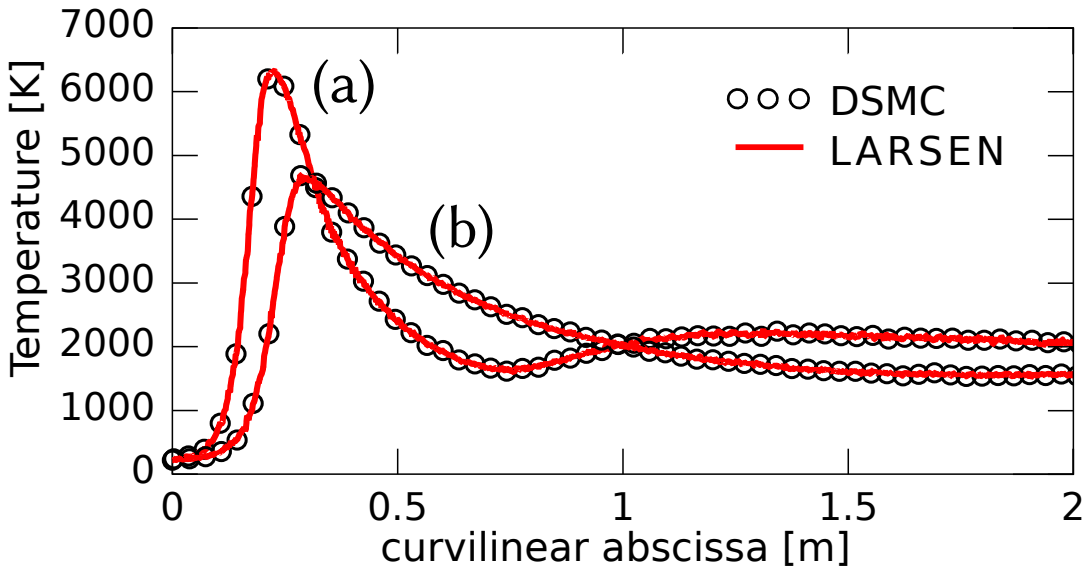


$\Longrightarrow$ System of ODEs

Hypersonic inert flow around a cylinder

- Axisymmetric DSMC simulation
- Pure argon
- $M = 10$
- $Kn = 0.05$





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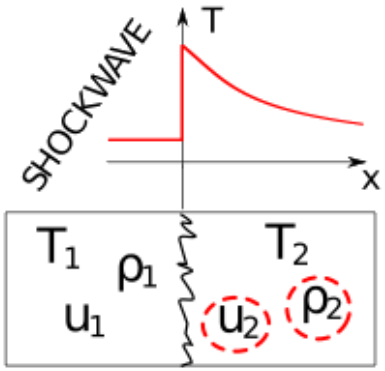
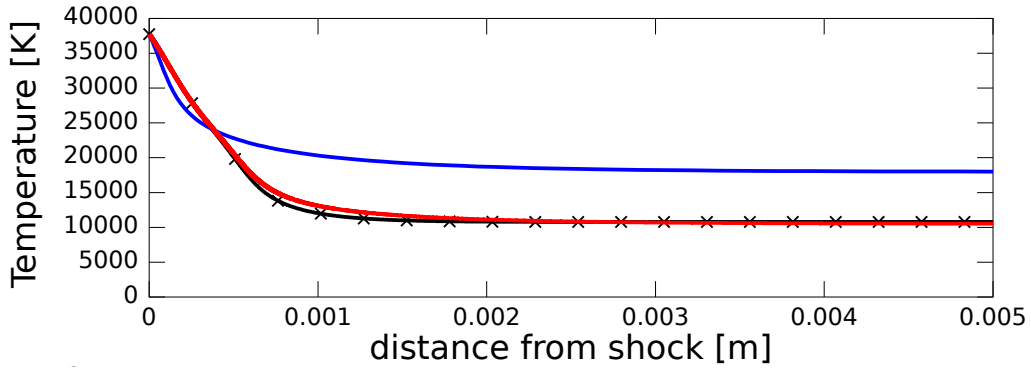
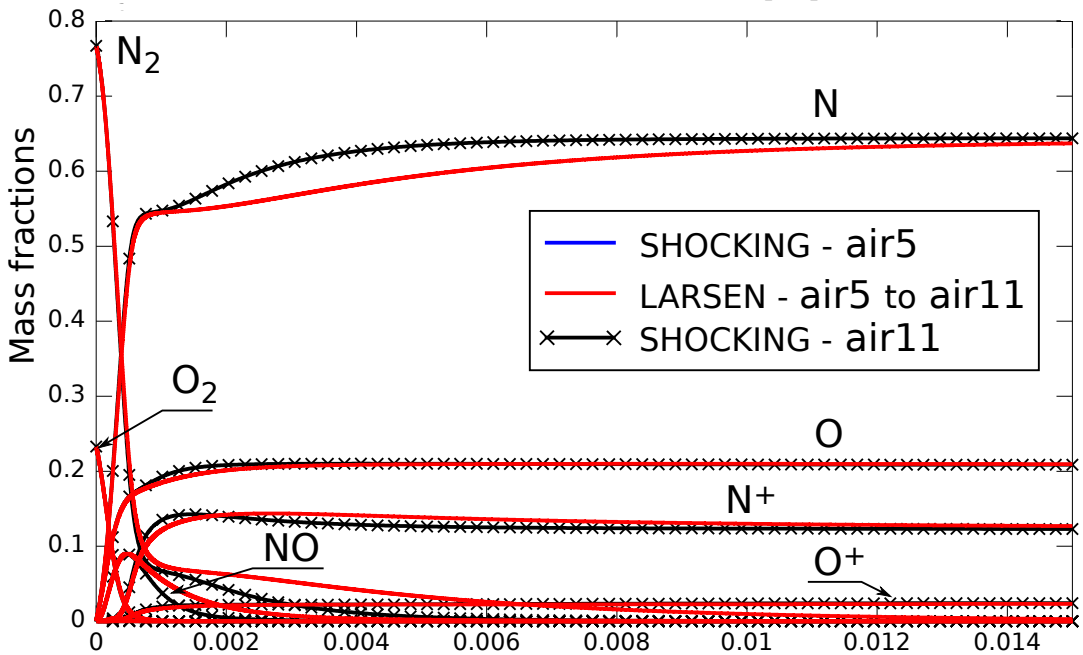
Relaxation behind a shock wave - refining chemistry

- Inviscid flow
- Fire-II capsule
  free-stream conditions
- air5: $N_2\ O_2\ N\ O\ NO$
- air11: air5 +
  $N^+\ O^+\ NO^+\ N_2^+\ O_2^+\ e^-$







T well predicted
ions concentrations well predicted
neutral species concentrations improved

Conclusions and future work

Conclusions

- Develop a **DSMC evaporation boundary condition** for silicates
- Couple flow-material-trajectory
- Develop a method to implement **detailed chemistry a posteriori**

Future work

- Include dynamic of molten layer to gas surface interactions
- Add **ionization of metallic species**
- Assess **recombination time** of free electrons in the trail

Thanks for your attention

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