

Settling of crystals in turbulent Rayleigh-Bénard convection

(work in progress)

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Content

- 1 Magmasphere
- 2 LBM
- 3 Chapman-Enskog
- 4 Maxey-Riley

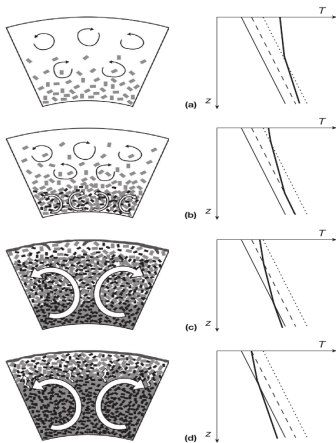
Early Earth

The Earth's mantle initially formed a magmasphere



- Accretion (no radiation: 3.75×10^5 K, full radiation: 70 K)
- Core segregation: $\Delta T \sim 1700$ K
- Moon forming impact: $T_{\text{final}} \sim 7000$ K
- Short lived isotopes (Al, K, ...)

Crystallization process



Onset of crystallization is given by intersection of the **adiabat** with the **liquidus** of magmasphere. **Lateral variations** are important too.

Rheological transition lies between the solidus and the liquidus (dashed curve).

From Solomatov (2015), ToG

Fractional vs equilibrium crystallization

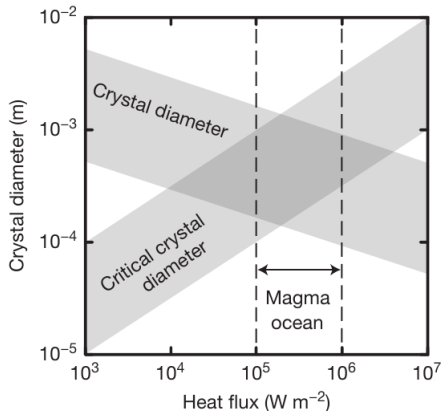


Figure 8 The crystal size during the early stages of crystallization of the magma ocean (assuming that it is controlled by nucleation in the downwelling flow) and the critical crystal size for suspension are shown as functions of the heat flux. The width of the curves (gray bands) represents the uncertainty range of one order of magnitude.

Magma dynamics

Governing equations

$$\begin{aligned}\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p / \rho_0 + \nu \nabla^2 \mathbf{u} - \alpha (T - T_0) \mathbf{g}, \\ \nabla \cdot \mathbf{u} &= 0, \\ \partial_t T + (\mathbf{u} \cdot \nabla) T &= \kappa \nabla^2 T.\end{aligned}$$

Non-dimensionalization

$$\begin{aligned}\mathbf{X} &= \mathbf{x}/H \\ \mathbf{U} &= \mathbf{u}/U_f \quad \text{with} \quad U_f = \sqrt{\alpha g \Delta T H} \\ \theta &= (T - T_0)/\Delta T\end{aligned}$$

$$\begin{aligned}\partial_\tau \mathbf{U} + (\mathbf{U} \cdot \nabla) \mathbf{U} &= -\nabla P + \sqrt{\frac{Pr}{Ra}} \nabla^2 \mathbf{U} + \theta \hat{\mathbf{z}} \\ \nabla \cdot \mathbf{U} &= 0 \\ \partial_\tau \theta + (\mathbf{U} \cdot \nabla) \theta &= \frac{1}{\sqrt{Pr Ra}} \nabla^2 \theta\end{aligned}$$

$$\sqrt{\frac{Pr}{Ra}} = \sqrt{\frac{\nu \nu \kappa}{\kappa \alpha g \Delta T H^3}} = \frac{\nu}{\sqrt{\alpha g \Delta T H}} = \frac{\nu}{U_f H} = \frac{1}{Re}$$

Ra of magma ocean

For the Rayleigh number one gets roughly ($\eta = 0.1$ Pa s)

$$Ra = \frac{\alpha g \Delta T H^3}{\kappa \nu} = \frac{5 \cdot 10^{-5} \cdot 9.8 \cdot 1 \cdot 2.89^3 \cdot 10^{18}}{5 \cdot 10^{-7} \cdot 2.5 \cdot 10^{-5}} \simeq 10^{27}.$$

and the Prandtl number $Pr = \nu/\kappa \simeq < 5, 50 >$.

A similar problem is faced in the MHD community when dealing with core dynamics.

CFD

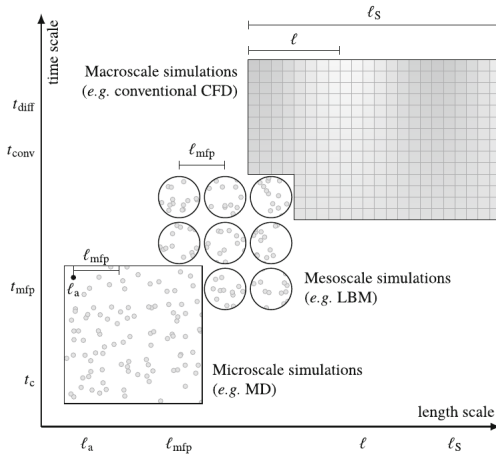


Fig. 1.3 The hierarchy of length and time scales in typical fluid dynamics problems. Depending on the level of details required, different simulation techniques are suitable

From Kruger et al. 2017 book: LBM principles and practice

Lattice gas automaton

$$\rho(\mathbf{x}, t) = \frac{m}{v_0} \sum_i n_i(\mathbf{x}, t) \quad \rho \mathbf{u}(\mathbf{x}, t) = \frac{m}{v_0} \sum_i \mathbf{c}_i n_i(\mathbf{x}, t)$$

v_0 is the volume of a node, m the mass of particles, $\mathbf{c}_i$ particle velocity, n_i is the occupation number (either 1 or 0)

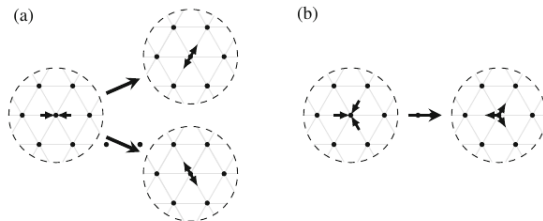
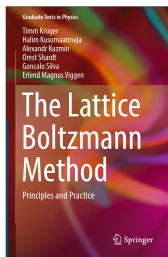
Collision: $n_i^*(\mathbf{x}, t) = n_i(\mathbf{x}, t) + \Omega_i(\mathbf{x}, t)$ with $\Omega_i \in -1, 0, 1$

Streaming: $n_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = n_i^*(\mathbf{x}, t)$

Evolution of the occupation number:

$$n_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = n_i(\mathbf{x}, t) + \Omega_i(\mathbf{x}, t)$$

Lattice gas automaton



Conservation of mass and momentum

$$\sum_i \Omega_i(\mathbf{x}, t) = 0 \quad \sum_i \Omega_i \mathbf{c}_i(\mathbf{x}, t) = \mathbf{0} \quad (1)$$

Boltzmann equation

The distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$:

$$\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \boldsymbol{\xi}, t) d^3\xi$$

$$\rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t) = \int \boldsymbol{\xi} f(\mathbf{x}, \boldsymbol{\xi}, t) d^3\xi$$

$$\rho(\mathbf{x}, t)E(\mathbf{x}, t) = \frac{1}{2} \int |\boldsymbol{\xi}|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d^3\xi$$

$$\rho(\mathbf{x}, t)e(\mathbf{x}, t) = \frac{1}{2} \int |\mathbf{v}|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d^3\xi$$

with $\mathbf{v} := \boldsymbol{\xi} - \mathbf{u}$

Boltzmann equation

By looking at how f changes along the trajectory of a particle $\mathbf{x}=\mathbf{x}(t) \Rightarrow f(\mathbf{x}, \boldsymbol{\xi}, t)=f(\mathbf{x}(t), \boldsymbol{\xi}(t), t)=f(t)$:

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t} \right) \frac{dt}{dt} + \left(\frac{\partial f}{\partial \mathbf{x}_\beta} \right) \frac{d\mathbf{x}_\beta}{dt} + \left(\frac{\partial f}{\partial \xi_\beta} \right) \frac{d\xi_\beta}{dt} \quad (2)$$

the Boltzmann equation is obtained:

$$\frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial \mathbf{x}_\beta} + \frac{F_\beta}{\rho} \frac{\partial f}{\partial \xi_\beta} = \Omega(f) \quad (3)$$

which is a partial differential equation for the evolution of f . Notice the similarity between (3) and the equation for the evolution of occupation number n_i in lattice gas models.

Mass conservation

From the microscopic conservation laws

$$\int \Omega(f) d^3\xi = 0$$

one can derive macroscopic conservation laws for the fluid,

$$\frac{\partial}{\partial t} \int f d^3\xi + \frac{\partial}{\partial x_\beta} \int \xi_\beta f d^3\xi + \frac{F_\beta}{\rho} \int \frac{\partial f}{\partial \xi_\beta} d^3\xi = \int \Omega(f) d^3\xi,$$

which gives the mass conservation law

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\beta}{\partial x_\beta} = 0 \quad \text{because} \quad \int \frac{\partial f}{\partial \xi_\beta} d^3\xi = 0$$

Momentum conservation

Similarly, from the microscopic (collision) momentum conservation

$$\int \xi \Omega(f) d^3\xi = \mathbf{0}$$

one can derive macroscopic momentum conservation:

$$\frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = -\frac{\partial}{\partial x_\beta} \int v_\alpha v_\beta f d^3\xi + F_\alpha \quad (4)$$

if the first RHS term is identified with the Cauchy stress tensor

$$\sigma_{\alpha\beta} = -\frac{\partial}{\partial x_\beta} \int v_\alpha v_\beta f d^3\xi. \quad (5)$$

The same can be done also for energy conservation, with heat flux defined as $q_\beta = -\frac{1}{2} \int v_\alpha^2 v_\beta f d^3\xi$

Equilibrium distribution

We may assume that the distribution function will reach an equilibrium distribution f^{eq} , isotropic in the velocity space around $\xi = \mathbf{u}$ and separable. In a reference frame moving with speed $\mathbf{u}$:

$$f^{\text{eq}}(|\mathbf{v}|^2) = f^{\text{eq}}(v_x^2 + v_y^2 + v_z^2) = f_{1D}^{\text{eq}}(v_x^2) f_{1D}^{\text{eq}}(v_y^2) f_{1D}^{\text{eq}}(v_z^2).$$

This alone is quite restrictive, with a solution

$$|\mathbf{v}| = \text{const} \quad \Rightarrow \quad f^{\text{eq}} = \text{const} \quad \Rightarrow \quad \ln f_{1D}^{\text{eq}}(v_x^2) = a + b v_x^2$$

$$f^{\text{eq}}(|\mathbf{v}|) = e^{3a} e^{b v^2}$$

and upon requiring the moments of f to give the density, momentum, energy of the fluid (by definition of f),

$$f^{\text{eq}}(\mathbf{x}, |\mathbf{v}|, t) = \rho \frac{3}{4\pi e} e^{-3v^2/4e} \quad \Rightarrow \quad f^{\text{eq}}(\mathbf{x}, |\mathbf{v}|, t) = \rho \frac{3}{4\pi e} e^{-3(\mathbf{v}-\mathbf{u})^2/4e}$$

i.e. the Maxwell-Boltzmann distribution

Euler equations

Exercise: assume that $f \simeq f^{\text{eq}}$ and EOS of ideal gas ($p = \frac{2}{3}\rho e$)

$$\frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = -\frac{\partial}{\partial x_\beta} \int v_\alpha v_\beta f \, d^3\xi + F_\alpha \quad (6)$$

gives

$$\frac{\partial}{\partial x_\beta} \int \frac{3\rho v_\alpha v_\beta}{4\pi e} e^{\frac{-3v^2}{4e}} d^3\xi = \frac{\partial(\frac{2}{3}\rho e)}{\partial x_\alpha} \Rightarrow \frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + F_\alpha$$

Similarly, the energy conservation obtains the form

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial(\rho e u_\beta)}{\partial x_\beta} = -p \frac{\partial u_\beta}{\partial x_\beta} \quad (7)$$

That means that viscous dissipation and thermal diffusivity are linked to dynamics of locally reaching the equilibrium distribution $f \rightarrow f^{\text{eq}}$

Chapman-Enskog theory

Performing perturbation theory on the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial x_\beta} + \frac{F_\beta}{\rho} \frac{\partial f}{\partial \xi_\beta} = \frac{1}{\epsilon} \Omega(f) \quad \left(= -\frac{1}{\tau} (f - f^{\text{eq}}) \right) \quad (8)$$

with ϵ being the Knudsen number, $Kn = l_{\text{mfp}}/l$. Taylor expansion of the solution $f = f(\epsilon)$

$$f = f^{\text{eq}} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + ..$$

BGK Collision operator

$$\Omega(f) := -\frac{1}{\tau} (f - f^{\text{eq}})$$

Chapman-Enskog

By inserting into eq. (8) and equating the same orders of ϵ , one gets, under approximation

$$\sigma_{\alpha\beta} = -\frac{\partial}{\partial x_\beta} \int v_\alpha v_\beta (f^{\text{eq}} + f^{(1)}) d^3\xi \quad (9)$$

that the Cauchy stress is equal to

$$\sigma = -p\mathbb{I} - (p\tau)(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

In other words, NVS are recovered, the viscosity being $\eta = p\tau$. Thermal diffusivity is related to the relaxation time as $\kappa = Rp\tau$.

Higher order gives Burnett model, ...

lattice Boltzmann equation

Recall lattice gas automaton

$$\rho(\mathbf{x}, t) = \frac{m}{v_0} \sum_i n_i(\mathbf{x}, t) \quad \rho \mathbf{u}(\mathbf{x}, t) = \frac{m}{v_0} \sum_i \mathbf{c}_i n_i(\mathbf{x}, t)$$

$$n_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = n_i(\mathbf{x}, t) + \Omega_i(\mathbf{x}, t)$$

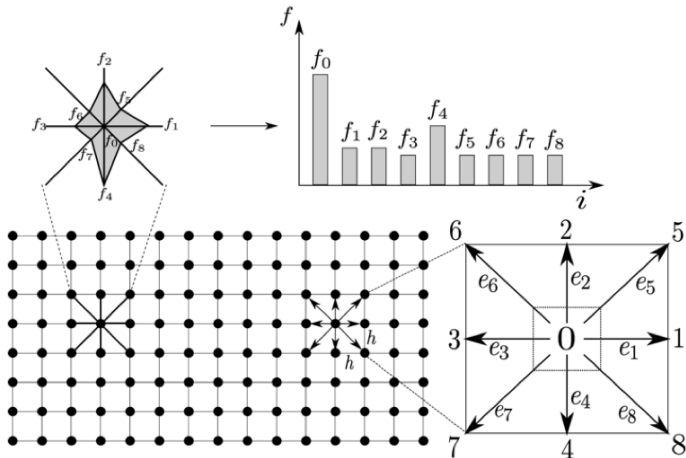
By discretizing the Boltzmann equation one gets (LBE)

$$\rho(\mathbf{x}, t) = \sum f_i(\mathbf{x}, t) \quad \rho \mathbf{u}(\mathbf{x}, t) = \sum \mathbf{c}_i f_i(\mathbf{x}, t)$$

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} (f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t))$$

$$f_i^{\text{eq}}(\mathbf{x}, t) = w_i \rho \left(1 + \frac{\mathbf{u} \cdot \mathbf{c}_i}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{c}_i)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{c_s^2} \right)$$

Discretization of the distribution function



Hermite polynomials

3.4.3.1 Definition and Construction of Hermite Polynomials

1D HPs are polynomials which can be obtained from the *weight function* (also called the *generating function*)

$$\omega(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}. \quad (3.22)$$

This weight function $\omega(x)$ allows us to construct the 1D HP of n -th order as

$$H^{(n)}(x) = (-1)^n \frac{1}{\omega(x)} \frac{d^n}{dx^n} \omega(x) \quad (3.23)$$

where $n \geq 0$ is an integer. The first six of these polynomials are

$$\begin{aligned} H^{(0)}(x) &= 1, & H^{(1)}(x) &= x, \\ H^{(2)}(x) &= x^2 - 1, & H^{(3)}(x) &= x^3 - 3x, \\ H^{(4)}(x) &= x^4 - 6x^2 + 3, & H^{(5)}(x) &= x^5 - 10x^3 + 15x. \end{aligned} \quad (3.24)$$

Hermite polynomials

Let us now apply the Hermite series expansion in (3.38) to the equilibrium distribution function f^{eq} in ξ -space:

$$f^{\text{eq}}(\rho, \mathbf{u}, \theta, \xi) = \omega(\xi) \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{a}^{(n),\text{eq}}(\rho, \mathbf{u}, \theta) \cdot \mathbf{H}^{(n)}(\xi), \quad (3.39)$$

$$\mathbf{a}^{(n),\text{eq}}(\rho, \mathbf{u}, \theta) = \int f^{\text{eq}}(\rho, \mathbf{u}, \theta, \xi) \mathbf{H}^{(n)}(\xi) \mathrm{d}^d \xi.$$

The substitution $\boldsymbol{\eta} = (\xi - \mathbf{u})/\sqrt{\theta}$ yields

$$\mathbf{a}^{(n),\text{eq}} = \rho \int \omega(\boldsymbol{\eta}) \mathbf{H}^{(n)}(\sqrt{\theta} \boldsymbol{\eta} + \mathbf{u}) \mathrm{d}^d \boldsymbol{\eta}. \quad (3.42)$$

These integrals can be directly computed, for example with the help of mathematical software packages:

$$\begin{aligned} a^{(0),\text{eq}} &= \rho, \\ a_{\alpha}^{(1),\text{eq}} &= \rho u_{\alpha}, \\ a_{\alpha\beta}^{(2),\text{eq}} &= \rho (u_{\alpha} u_{\beta} + (\theta - 1) \delta_{\alpha\beta}), \\ a_{\alpha\beta\gamma}^{(3),\text{eq}} &= \rho \left[u_{\alpha} u_{\beta} u_{\gamma} + (\theta - 1) (\delta_{\alpha\beta} u_{\gamma} + \delta_{\beta\gamma} u_{\alpha} + \delta_{\gamma\alpha} u_{\beta}) \right]. \end{aligned} \quad (3.43)$$

Maxey-Riley

$$\frac{d\mathbf{v}}{dt} = \beta \frac{D\mathbf{u}}{Dt} + \frac{1}{\tau_D}(\mathbf{u} - \mathbf{v}) + (1 - \beta)\mathbf{g} \quad (10)$$

The parameters in this equation of motion are:

$\beta = 3\rho_f/(\rho_f + 2\rho_p)$ the modified density ratio

$\tau_D = R^2/(3\nu\beta)$ where R is the particle radius

$$\frac{d\mathbf{V}}{d\tau} = \beta \frac{D\mathbf{U}}{D\tau} + \frac{1}{St_H}(\mathbf{U} - \mathbf{V}) + \Lambda \hat{\mathbf{z}} \quad (11)$$

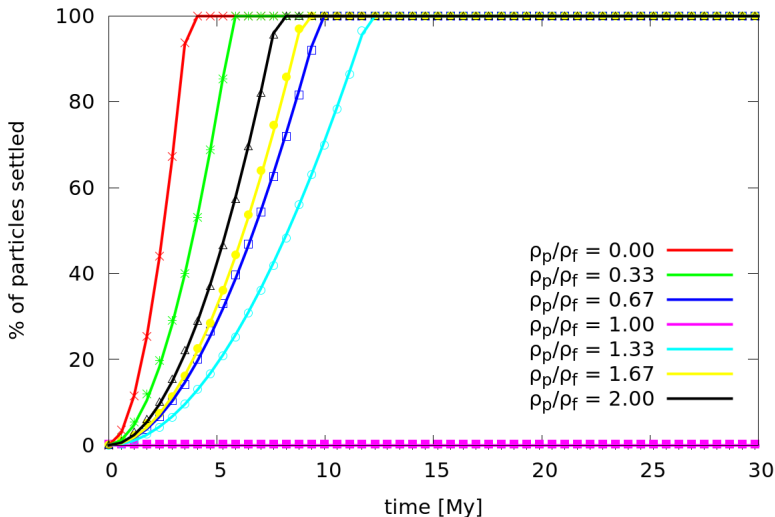
with the dimensionless control parameters:

$$\beta = 3\rho_f/(\rho_f + 2\rho_p)$$

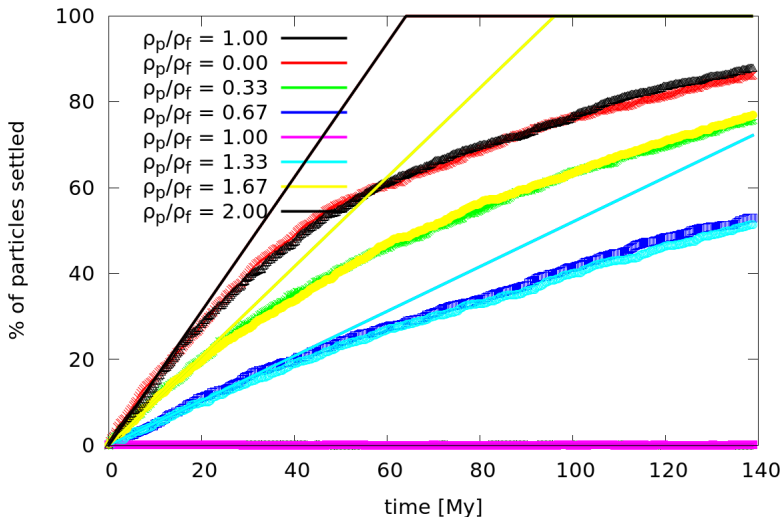
$$St_H = \tau_D/\tau_H = R^2\sqrt{\alpha g \Delta T}/(3\nu\beta\sqrt{H})$$

$$\Lambda = (\beta - 1)/(\alpha \Delta T)$$

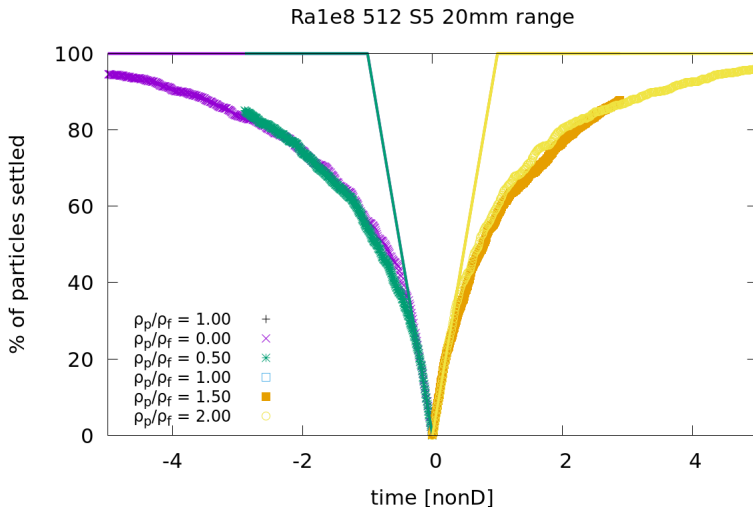
Results - big particles



Results - small particles



Results - rescaled by terminal velocity



Results - bubble capture

