Rarefied gas flow into vacuum through a long circular pipe composed of two sections of different radii

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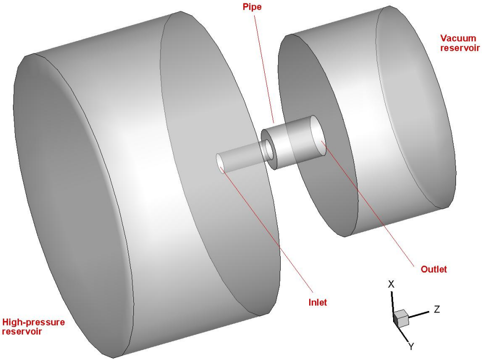
Specification of the problem

- Consider two (infinitely) large reservoirs filled with the same monatomic gas and connected by a pipe of length L. The first half of the pipe is of radius R_1. The second half, adjacent to the vacuum region, is of the radius $R_2 \geq R_1$.
- The complete accommodation of momentum and energy of molecules occurs at the pipe surface, which is kept under the constant temperature T_1.
- An example of geometry of the problem is shown here for $L/R_1 = 10$ and $R_2/R_1 = 2$.



BKE with the Shakhov model collision integral (1968)

- The 3D S-model equation for the velocity distribution function f is given by

$$\xi_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{p}{\mu}(f^+ - f), \quad f^+ = f_M \left[1 + \frac{4}{5}(1-\mathrm{Pr})\, S_\alpha c_\alpha \left(c^2 - \frac{5}{2}\right)\right],$$

$$f_M = \frac{n}{(2\pi R_g T)^{3/2}} \exp(-c^2), \quad S_i = \frac{1}{n}\int c_i c^2 f d\boldsymbol{\xi}, \quad \boldsymbol{c} = \frac{\boldsymbol{v}}{\sqrt{2R_g T}}, \quad c^2 = c_\beta c_\beta.$$

- Macroscopic quantities defined as

$$n = \int f d\boldsymbol{\xi}, \quad n\boldsymbol{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi}, \quad \frac{3}{2} mnR_g T + \frac{1}{2} mnu^2 = \frac{1}{2} m \int \xi^2 f d\boldsymbol{\xi},$$

$$\boldsymbol{q} = \frac{1}{2} m \int \boldsymbol{v} v^2 f\, d\boldsymbol{\xi}, \quad \boldsymbol{v} = \boldsymbol{\xi} - \boldsymbol{u}, \quad \rho = mn, \quad p = \rho R_g T,$$

$$u^2 = u_\alpha u_\alpha, \quad v^2 = v_\alpha v_\alpha, \quad \xi^2 = \xi_\alpha \xi_\alpha, \quad d\boldsymbol{\xi} = d\xi_x d\xi_y d\xi_z.$$

- Boundary condition on the surface:

$$f_w = \frac{n_w}{(2\pi R_g T_{\mathrm{sur}})^{3/2}} \exp\left(-\frac{\xi^2}{2R_g T_{\mathrm{sur}}}\right), \quad n_w = \sqrt{\frac{2\pi}{R_g T_{\mathrm{sur}}}} N_i, \quad N_i = -\int_{\xi_n<0} \xi_n f d\boldsymbol{\xi}.$$

- Here Prandtl number $\mathrm{Pr} = 2/3$, R_g is gas constant, m is molecular mass.

Non-dimensional form of the S-model equation

- Let us pass to non-dimensional variables as follows:

$$\mathbf{x}' = \frac{\mathbf{x}}{R_1}, \quad n' = \frac{n}{n_1}, \quad p' = \frac{p}{p_1}, \quad T' = \frac{T}{T_1},$$

$$\mathbf{u}' = \frac{\mathbf{u}}{v_*}, \quad \boldsymbol{\xi}' = \frac{\boldsymbol{\xi}}{v_*}, \quad \mathbf{q}' = \frac{\mathbf{q}}{m n_1 v_*^3}, \quad f' = \frac{f}{n_1 v_*^3}.$$

  where $p_1 = m n_1 R_g T_1$, $v_* = \sqrt{2 R_g T_1}$

- The degree of gas rarefaction is described by the so-called rarefication parameter δ_1, which is inversely proportional to the Knudsen number:

$$\delta = \frac{R_1 p_1}{\mu(T_1) v_*} = \frac{8}{5\sqrt{\pi}} \frac{1}{\mathrm{Kn}}, \quad \mathrm{Kn} = \frac{\lambda_1}{R_1}.$$

  Here λ_1 is the free molecular path at reference conditions.

- Below the non-dimensional variables are denoted by the same symbols as dimensional ones.

- In the non-dimensional variables the kinetic equation takes the form:

$$\xi_x \frac{\partial f}{\partial x} + \xi_y \frac{\partial f}{\partial y} + \xi_z \frac{\partial f}{\partial z} = \nu(f^{(S)} - f), \quad \nu = \frac{nT}{\mu(T)}\delta_1,$$

$$f^{(S)} = f_M \left(1 + \frac{4}{5}(1-\mathrm{Pr})\boldsymbol{Sc}(c^2 - \frac{5}{2})\right), \quad f_M = \frac{n}{(\pi T)^{3/2}} e^{-c^2}, \quad \boldsymbol{S} = \frac{2\boldsymbol{q}}{nT^{3/2}}.$$

- Macroscopic quantities defined as

$$\left(n, n\boldsymbol{u}, \frac{3}{2}nT + nu^2, \boldsymbol{q}\right) = \int \left(1, \boldsymbol{\xi}, \xi^2, \frac{1}{2}\boldsymbol{v}v^2\right) f d\boldsymbol{\xi}.$$

  The non-dimensional pressure is given by $p = nT$.

- Boundary condition on the surface:

$$f(\boldsymbol{x}, \boldsymbol{\xi}) = f_w = \frac{n_w}{(\pi T_w)^{3/2}} \exp\left(-\frac{\xi^2}{T_w}\right), \quad \xi_n = (\boldsymbol{\xi}, \mathbf{n}) > 0,$$

$$n_w = N_i / N_r, \quad N_i = -\int\limits_{\xi_n<0} \xi_n f d\boldsymbol{\xi}, \quad N_r = +\int\limits_{\xi_n>0} \xi_n \frac{1}{(\pi T_w)^{3/2}} \exp\left(-\frac{\xi^2}{T_w}\right) d\boldsymbol{\xi}.$$

Numerical method of solution & Nesvetay-3D package

- Discrete velocity method conservative with respect to collision integral
  - Steady solution is found by time marching
  - Time-dependent calculations: Kolgan-type (1972) TVD method
  - Conservative calculations of macroscopic variables (number density, velocity, temperature, heat flux vector)
- Fully implicit time marching
  - One-step linearized method with large CFL numbers $\approx 10 \ldots 1000$
  - LU-SGS approach of Men'shov and Nakamura to compute time increments
- Second-order accurate Total Variation Diminishing method
  - Arbitrary cells in physical domain
  - Least-square or quasi-1D reconstructions
  - Various slope limiters
- Parallel solver
  - Both physical or velocity domains can be split
  - Calculations run on up to 512 CPU cores

Conservative discrete velocity framework

- March in time to steady state:

$$\frac{\partial}{\partial t} f = -\boldsymbol{\xi} \nabla f + J(f), \quad J = \nu(f^{(S)} - f),$$

- Replace the infinite domain of integration in the molecular velocity space $\boldsymbol{\xi}$ by a finite computational domain.
- Let $\boldsymbol{\Xi}_k$ be a vector, made of k-th component of velocity nodes over the whole mesh:

$$\boldsymbol{\Xi}_k = (\xi_{k1}, \xi_{k2}, \xi_{k3}, \ldots \xi_{kN_\xi})^T.$$

- The kinetic equation is replaced by a system of N_ξ advection equations:

$$\frac{\partial}{\partial t} \boldsymbol{f} + \frac{\partial}{\partial x_\alpha} (\boldsymbol{\Xi}_\alpha \circ \boldsymbol{f}) = \boldsymbol{J}, \quad \boldsymbol{J} = \nu(\boldsymbol{f}^{(S)} - \boldsymbol{f}).$$

  Here operation $\circ$ corresponds to a component by component multiplication of vectors $c = a \circ b \quad \rightarrow \quad c_i = a_i b_i$.

One step implicit numerical method

- Denote by $|V_i|$ the cell volume, $|A|_{il}$ area of face l. Integration over a control volume and use of calculus leads to the following implicit method:

$$\frac{\Delta \boldsymbol{f}_i}{\Delta t} = \boldsymbol{R}_i^{n+1}, \quad \Delta \boldsymbol{f}_i = \boldsymbol{f}_i^{n+1} - \boldsymbol{f}_i^{n}, \quad \boldsymbol{R}_i^{n+1} = -\frac{1}{|V_i|} \sum_{l=1} \boldsymbol{\Phi}_{il}^{n+1} + \boldsymbol{J}_i^{n+1},$$

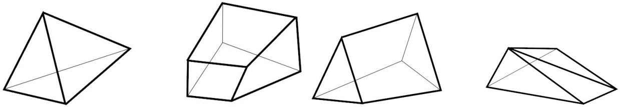
  where $\boldsymbol{f}_i^n = \boldsymbol{f}(t^n, \boldsymbol{x}_i)$ - spatial average of distribution function in spatial cell V_i at time moment t^n.

- The numerical flux through the face A_{il} is defined as

$$\boldsymbol{\Phi}_{il}^{n+1} = \int\limits_{A_{il}} (\boldsymbol{\xi}_{nil} \circ \boldsymbol{f}^{n+1}) ds, \quad \boldsymbol{\xi}_{nil} = n_{1l}\boldsymbol{\Xi}_1 + n_{2l}\boldsymbol{\Xi}_2 + n_{3l}\boldsymbol{\Xi}_3.$$

  Here vector $\boldsymbol{\xi}_{nl}$ consists of projections of velocity nodes onto outward unit normal $\boldsymbol{n}_{il}$ of face l of cell V_i.

- We consider cells of various shapes.



Linearization of the implicit scheme

- For the collision term
$$\boldsymbol{J}_i^{n+1} \approx \boldsymbol{J}_i^n - \nu_i^n \Delta \boldsymbol{f}_i.$$
- For the flux assume first-order spatial approximation while computing Jacobians:
$$\boldsymbol{\Phi}_{il}^{n+1} \approx \boldsymbol{\Phi}_{il}^n + \frac{\partial \boldsymbol{\Phi}_{il}^n}{\partial \boldsymbol{f}_i^n} \circ \Delta \boldsymbol{f}_i + \frac{\partial \boldsymbol{\Phi}_{il}^n}{\partial \boldsymbol{f}_{i_l}^n} \circ \Delta \boldsymbol{f}_{i_l}.$$
- Important: $\boldsymbol{\Phi}_{il}^n$ is computed with the full second order of spatial accuracy.
- Regrouping, we get:
$$\left(\left(\frac{1}{\Delta t} + \nu_i^n \right) \boldsymbol{I}_\xi + \frac{1}{|V_i|} \sum_{l=1} \frac{\partial \boldsymbol{\Phi}_{il}^n}{\partial \boldsymbol{f}_i^n} \right) \circ \Delta \boldsymbol{f}_i + \frac{1}{|V_i|} \sum_{l=1} \left(\frac{\partial \boldsymbol{\Phi}_{il}^n}{\partial \boldsymbol{f}_{i_l}^n} \right) \circ \Delta \boldsymbol{f}_{i_l} = \boldsymbol{R}_i^n.$$

  Here $\boldsymbol{I}_\xi = \mathrm{diag}(1, \ldots, 1)^T$ is a unit matrix of dimension N_ξ.
- These relations connect increments of the solution in the cell V_i and its neighbours for all cells $i = 1, \ldots, N_{\mathrm{space}}$.
- The system is solved using an adaptation of the LU-SGS algorithm of Men'shov & Nakamura (2000). Details omitted.

Computed reduced flow rate data

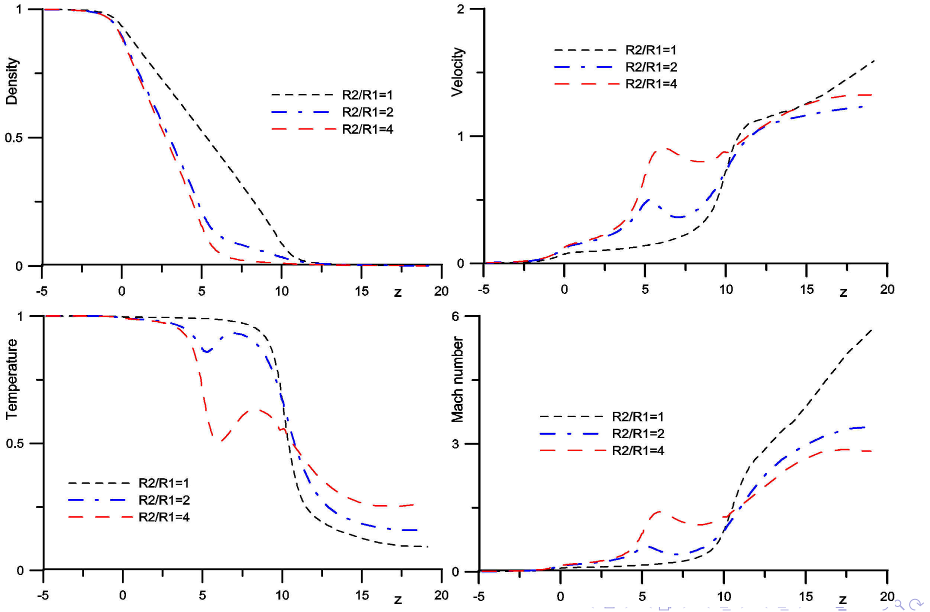
Reduced flow rate $Q = \dfrac{\dot{M}}{\dot{M}_0}, \quad \dot{M}_0 = \sqrt{\pi}/2, \quad \dot{M} = \int\limits_{A(z)} n(x,y,z)u_3(x,y,z)dxdy.$

	$R_2=1$				$R_2=2$			$R_2=4$
	Ref. 1		Ref. 2		Present work			
δ_1	$L=5$	$L=10$	$L=10$	$L=20$	$L=5$	$L=10$	$L=20$	$L=10$
0.	0.311	0.192	0.190	0.108	0.446	0.291	0.177	0.309
0.1	0.312	0.190	0.191	0.123	0.452	0.295	0.177	0.312
1	0.334	0.198	0.201	0.127	0.499	0.318	0.185	0.337
10	0.543	0.335	0.335	0.220	0.770	0.525	0.316	0.542
20	0.695	0.463	0.462	0.320	0.919	0.684	0.446	0.691
50	0.917	0.696	0.697	0.550	1.104	0.909	0.688	0.916
100	1.068	0.874	0.889	0.773	1.221	1.060	0.876	1.069

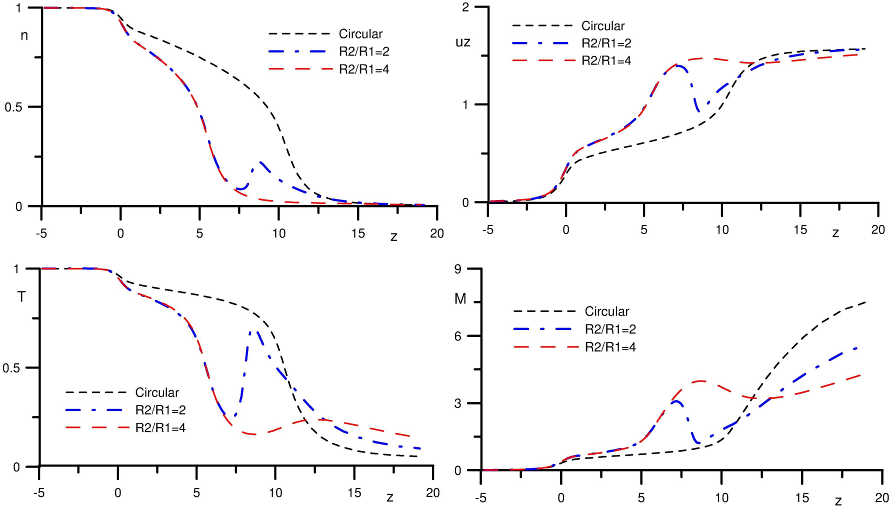
Ref 1: S. Varoutis et al. Rarefied gas flow through short tubes into vacuum. *J. Vac. Sci. Technol.*, 26(1):228–238, 2008.

Ref 2: V.A. Titarev et. al. Rarefied gas flow through a diverging conical pipe into vacuum. *Vacuum*, 101:10–17, 2014.

Axial plots for $L = 10$ and $\delta_1 = 1$.

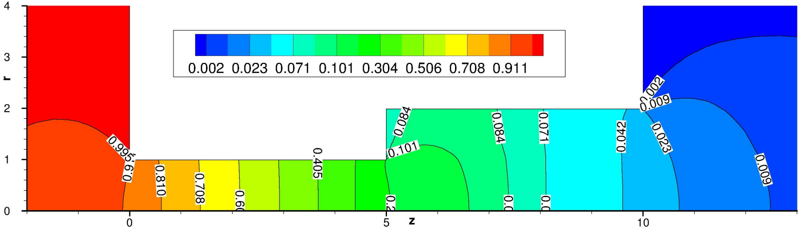


Axial plots for $L = 10$ and $\delta_1 = 100$.

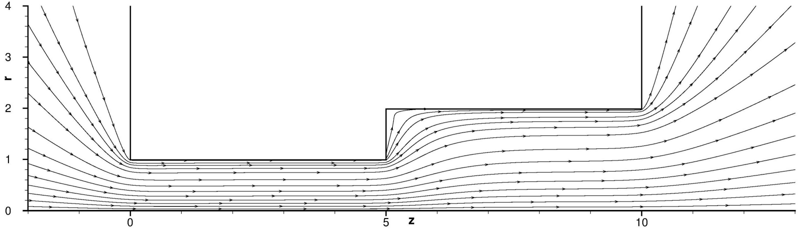


Contour lines for $\delta_1 = 1$.

Number density:

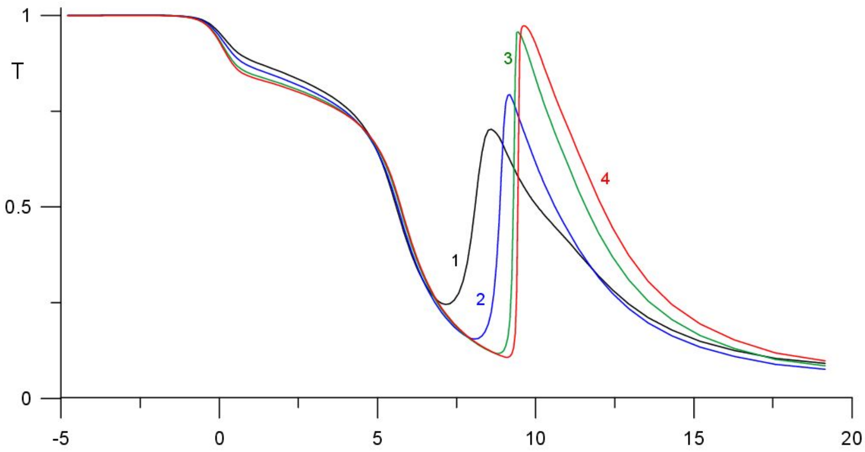


Stream lines:



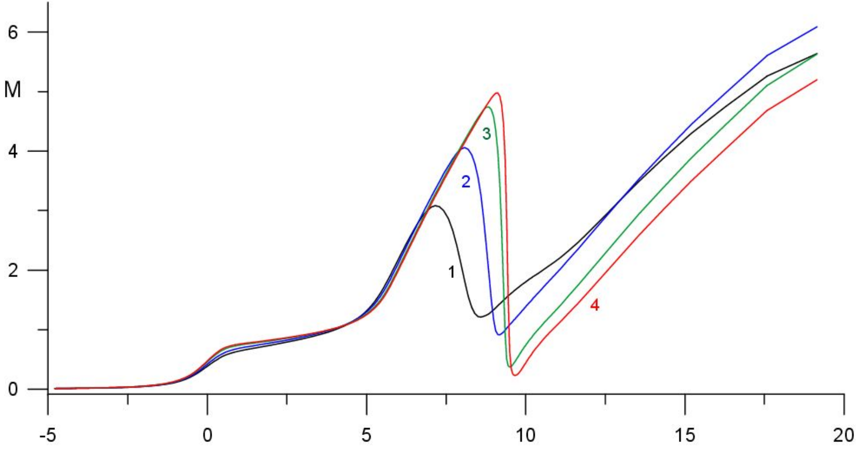
Formation of a Mach disk (1)

Axial distribution of temperature: curves 1–4 correspond to $\delta_1 = 100$, 200, 500, 1000.



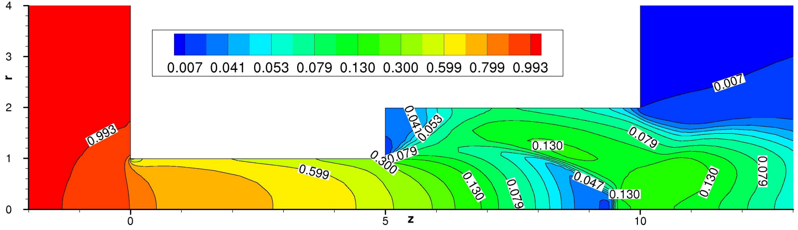
Formation of a Mach disk (2)

Axial distribution of Mach number: curves 1–4 correspond to $\delta_1 = 100, 200, 500, 1000$.

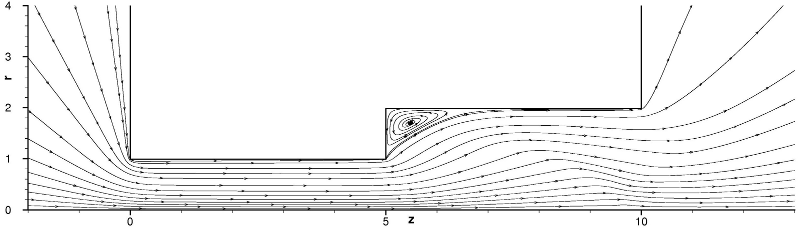


Formation of a Mach disk: contour lines for $\delta_1 = 1000$.

Number density:

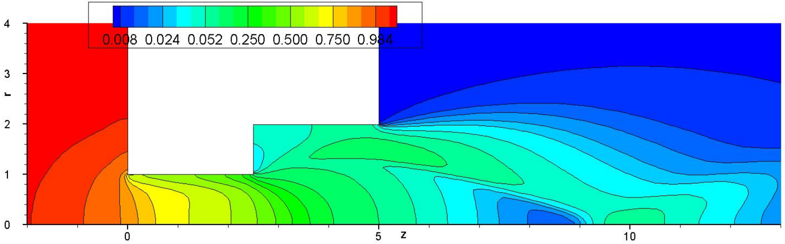


Stream lines:

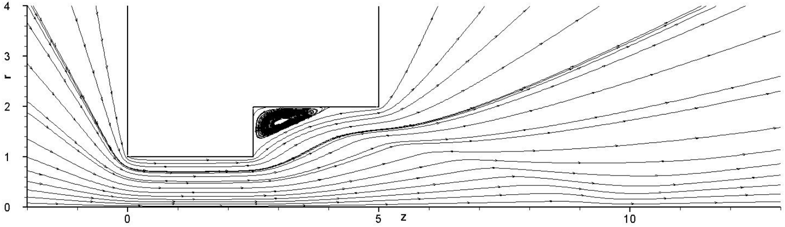


Formation of a Mach disk for $L = 5$ & $\delta_1 = 1000$.

Number density:



Stream lines:



Conclusions

Some recent publications for 3D rarefied gas flows:

1. V.A. Titarev and E.M. Shakhov. Computational study of a rarefied gas flow through a long circular pipe into vacuum //*Vacuum, Special Issue "Vacuum Gas Dynamics"*. 2012. V. 86. N. 11. p. 1709-1716.
2. V.A. Titarev, E.M. Shakhov, and S.V. Utyuzhnikov. Rarefied gas flow through a diverging conical pipe into vacuum // *Vacuum*, 101:10–17, 2014.
3. V. Titarev, M. Dumbser and S. Utyuzhnikov. Construction and comparison of parallel implicit kinetic solvers in three spatial dimensions // *J. Comp. Phys.* 2014. V. 256. p. 17-33.
4. V.A. Titarev and E.V. Shakhov. Rarefied gas flow into vacuum through a pipe composed of two circular sections of different radii // *Vacuum.* 2014, in press.
5. V.A. Titarev. Computer package Nesvetay-3D for modelling three-dimensional flows of monatomic rarefied gases // *Science & Education*. 2014. N. 6.

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