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High Vacuum Gas Pumping and Boundary Coupling

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1) Introduction

2) Molecular flow

3) The circular junction

4) The simple obstruction

5) Conclusion and perspective

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Abstract or Executive summary:

The gas flow in the low pressure limit, named molecular flow regime, is practically important for many scientific instruments and is a case of transport with zero viscosity, of great theoretical importance.

As an alternative to Monte Carlo methods typically used to estimate pipe conductance, an integral boundary equation (IBE) is here discussed, and solved, at least for simple 2D geometries (a circular junction and a simple pipe obstruction).

An ad hoc algorithm to find obstacles on the view lines was developed for the latter case. The particular cares requested at the corners and in the interpolation from boundary to inner domain are shown. Relation between flow and pressures at ports is discussed, with the usual cosine law for the distribution of the velocities at input. For the circular junction, a typical PDE (partial differential equation) is here shown to have the same solution of the IBE, which allows for a comparison of the numerical precision of both approaches, showing a good agreements.

1) INTRODUCTION:

Many scientific instruments depends on high vacuum equipment

Calculation of gas pressure p in vacuum chamber or in connecting pipes is very important!

We have two different regimes, depending on the Knudsen number Kn instead of Reynold number Re

$$K_n = D/\lambda \qquad R_e = \rho v_F D/\eta \qquad (1)$$

where D [m] is a typical diameter of the gas pipe, v_F the average velocity of the gas (fluid), ρ is the mass density (typically proportional to pressure), η [Pa s] is the (dynamic) viscosity and λ [m]is the mean free path of molecules

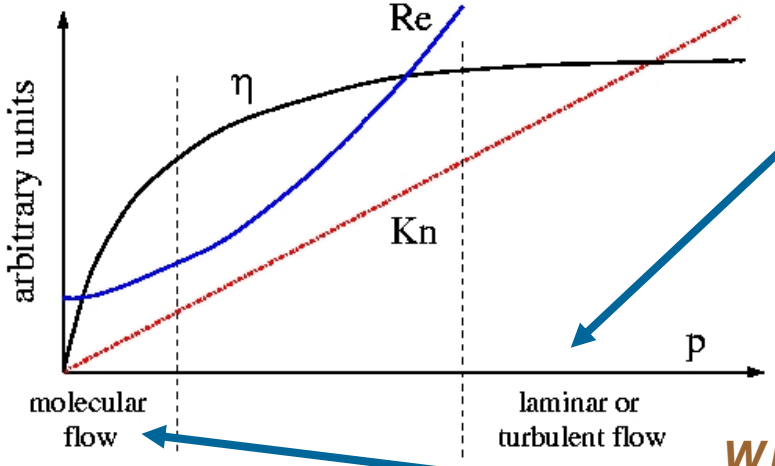


Fig 1: Kn vs Pressure p

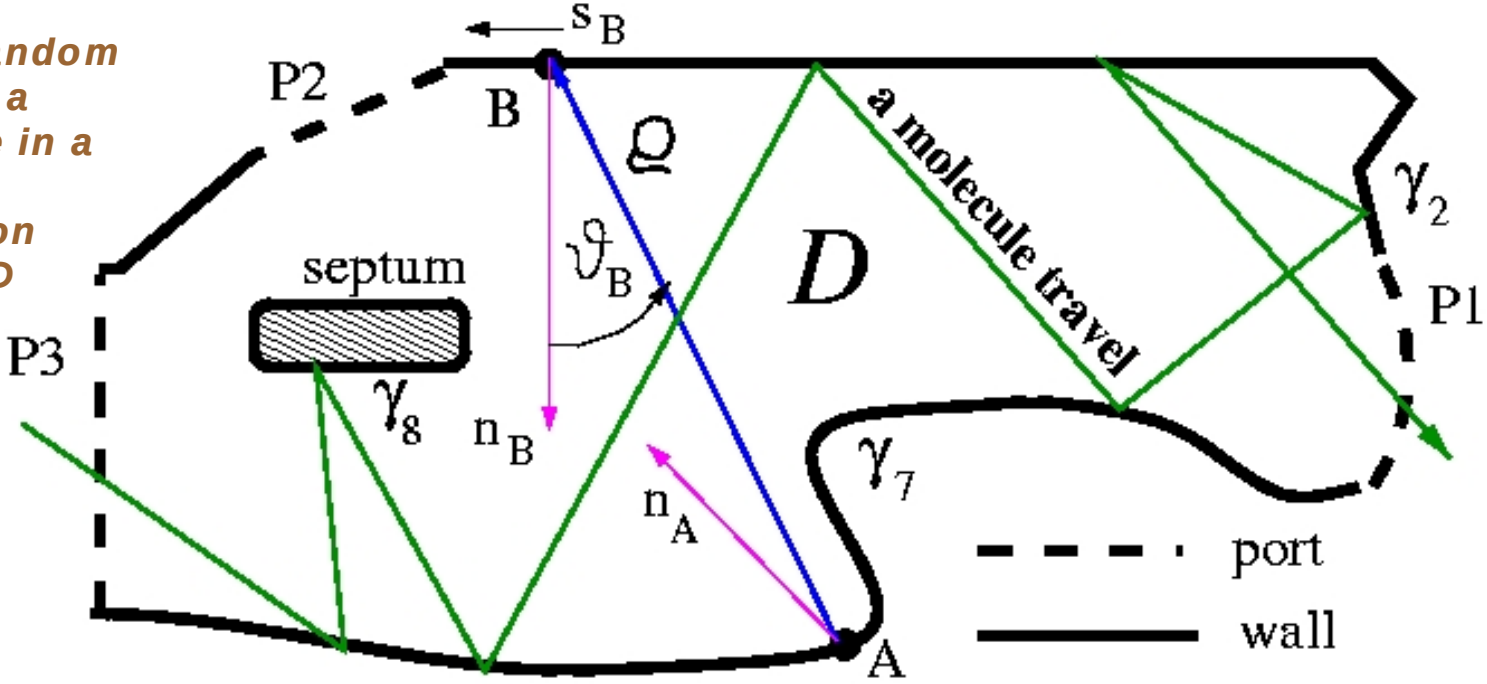
When Kn > 80, we have the viscous regime, where we can apply the compressible Navier Stokes equations

When Kn < 3, we have the molecular flow, here discussed

2) MOLECULAR FLOW

Definition of molecular flow regime: the frequence of molecule collisions among themselves is neglected compared to the collisions with walls, since λ is large (compared to size D)

Fig2 A random travel of a molecule in a generic simulation domain D



At wall, molecules lose a large fraction of their momentum, and they may bounce back immediately or stick to wall and be reemitted after a while. In any case, we assume they all get reemitted (in stationary regime) with an angular distribution (for $\vartheta_B < \pi/2$)

$$f(\vartheta_B) = \frac{1}{2}\cos\vartheta_B \quad \textit{in 2D or} \quad f(\vartheta_B) = \frac{1}{\pi}\cos\vartheta_B \quad \textit{in 3D} \qquad (2)$$

For simplicity let gas temperature T and wall temperature be uniform (T=isothermal), so that $p=n\,k_B T$. Then the density n^{reem} of reemitted molecules at point A (the density n^{inci} of the flow of incident molecules) is the unknown in the mass balance at wall equation

$$n^{\text{reem}}\frac{v_{av}}{4}=n^{\text{inci}}\frac{v_{av}}{4}+\frac{F^{\text{vo}}}{k_B T}\qquad v_{av}=\sqrt{\frac{8\,k_B T}{\pi\,m}}\qquad (3)$$

and the net volumetric input flow density F^{vo} [Pa m/s] is the driving data (nonzero only on ports) and v_{av} is the mean of gas molecule speed.

With the definition incident pressure $p^{in}=n^{inci}\,k_B T$ and reemitted flow equivalent pressure $p^{re}=n^{reem}\,k_B T$ and $F^{ins}=4\,F^{vo}/v_{av}$ we get the boundary equation:

$$p^{re}=F^{ins}+p^{in}\qquad (4)$$

with the coupling

$$p^{in}(A)=L\left[p^{re}\right]\equiv\int ds_B\,\frac{\cos\vartheta_A\cos\vartheta_B}{2r}\,p^{re}(B)I_{AB}\qquad (5)$$

where $I_{AB}=1$ if A and B sees each other and $I_{AB}=0$ otherwise. We also define the inner pressure for postprocessing only:

$$p^{i}(A)=M\left[p^{re}\right]\equiv\int ds_B\,\frac{\cos\vartheta_B}{2\pi\,r_{AB}}\,p^{re}(B)I_{AB},\quad A\notin\partial D\qquad (6)$$

with D the solution domain

2.2) IMPLEMENTATION:

Implementation of the integral boundary equation (IBE) eqs 4 and 5 in COMSOL weak boundary mode is straightforward. On walls and some ports P3 we set

```
bnd.weak = 'test(pre)*(elle+fins-pre)';
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(7)

where "elle" is the integration coupling variable representing the eq 5. On port P1 either :

we impose p^{re} as a fixed boundary condition

or we set $p^{re}=p_1$ with p_1 a global variable, to be solved with the condition of obtaining a fixed flow F^{ins}

Observation: COMSOL translate eq (4,5) to a stiffness matrix K and solve it, as it does fo any PDE. There are 2 differences:

a) the PDE stiffness matrix is sparse, while the stiffness matrix of eqs. (4,5) is rather dense Both assemblying and solution time are longer at equal dof number.

b) eq (4) involves fewer dof than a 2D PDE model in the same geometry

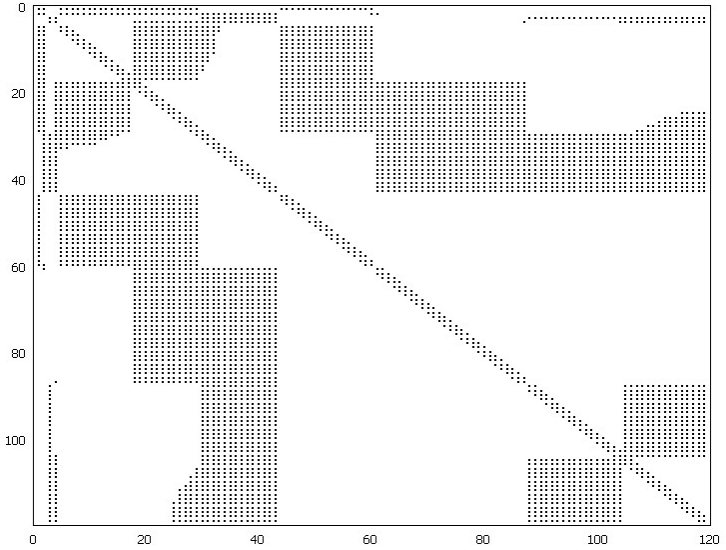


Fig 3: dots are nonzero K elements

Comparison with other solution methods:

the traditional computation method of molecular flow is the Montecarlo (MC), that is travels of one million molecules are followed; at each wall collision, a new molecule velocity is randomly selected with distribution (1). There are two disadvantages:

a) MC is computationally expensive

b) toolboxes for MC have rapidly changing user interfaces (or request C++ programming), to my knowlegde

Comparison with similar problems:

a) rendering illumination in room (so called radiosity problem). The reemitted light L^{re} is a fraction f of incident light L^{in}, plus a driving source L^S (sun or a lamp):

$$L^{re} = f\ L^{in} + L^S \qquad (8)$$

which is similar to eq 4. Moreover coupling eq 5 is equal.

b) T^4 radiation surface to surface (see COMSOL heat transfer module, radiosity). In that case, incident heat can be reemitted or conducted Q^C through solid bodies and two sides of a thin wall interact. On walls:

$$Q^{re} = Q^{in} - Q^C \qquad (9)$$

3) RESULTS FOR THE CIRCULAR JUNCTION

The simpler vacuum chamber to study is a circle. We consider two or four ports (P1, P2, P3, P4).

To get a first idea of the results let us look to inner pressure, which is near the average of input and output pressuse in most of domain D

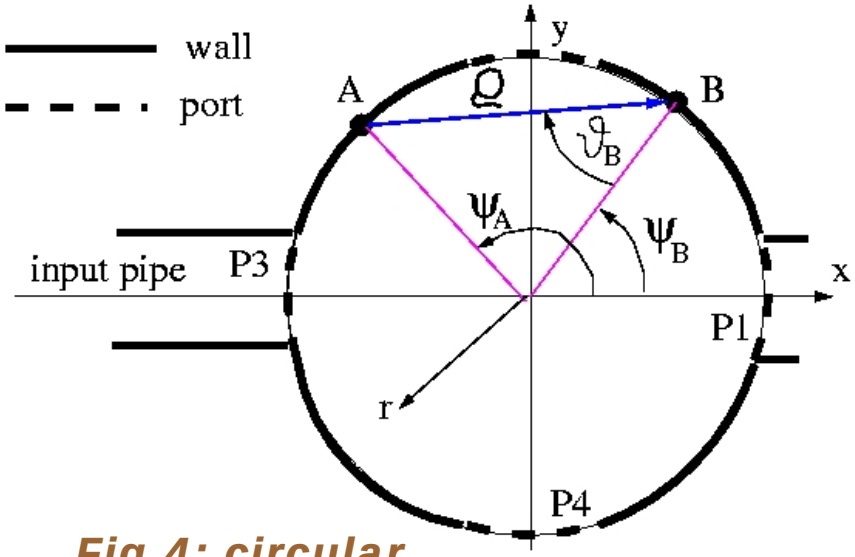


Fig 4: circular junction

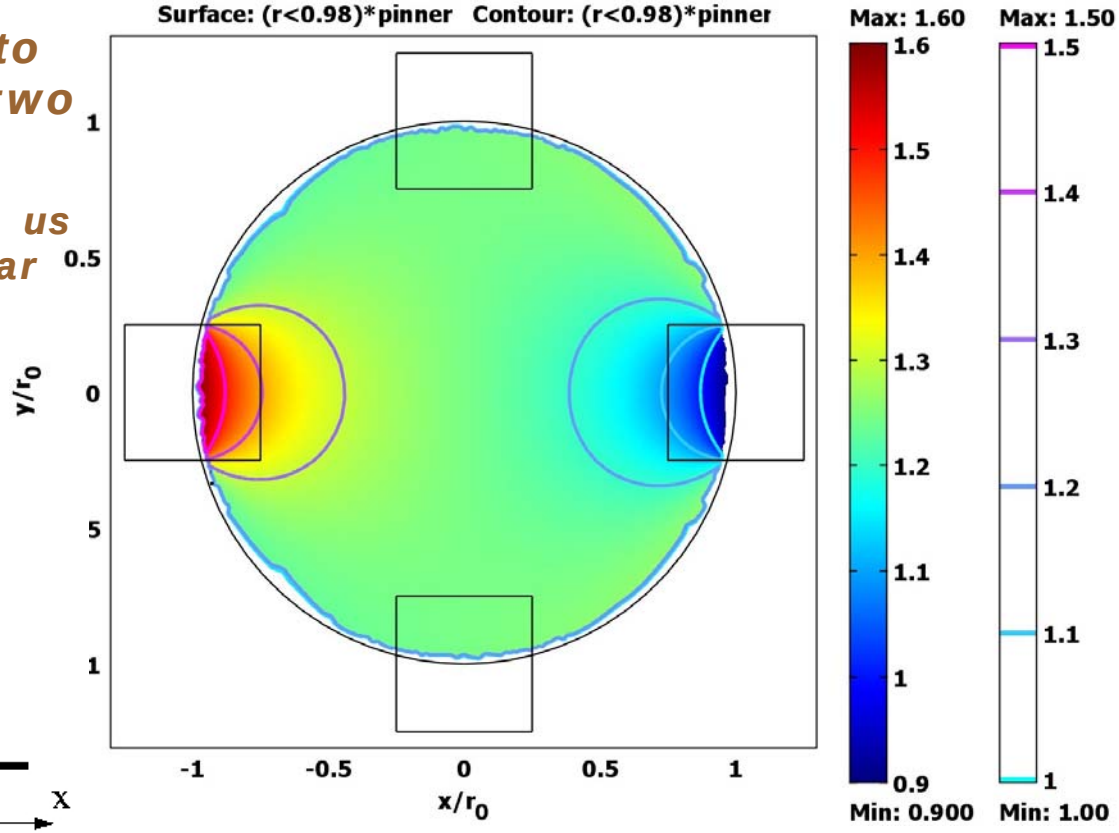


Fig 5: Simulation 'II' results: contour and surface plot of p^i for an inner region r<0.98 r0.

Here p_3=2 mPa and p_1=0.5 mPa, with the result F^{ins}= 0.825 mPa (at P3) and p_0=1.25 mPa

A detail of pressure at wall shows that incident pressure is slightly lower near input (and anyway is roughly constant): indeed input P3 irradiates output side x>0 more than itself

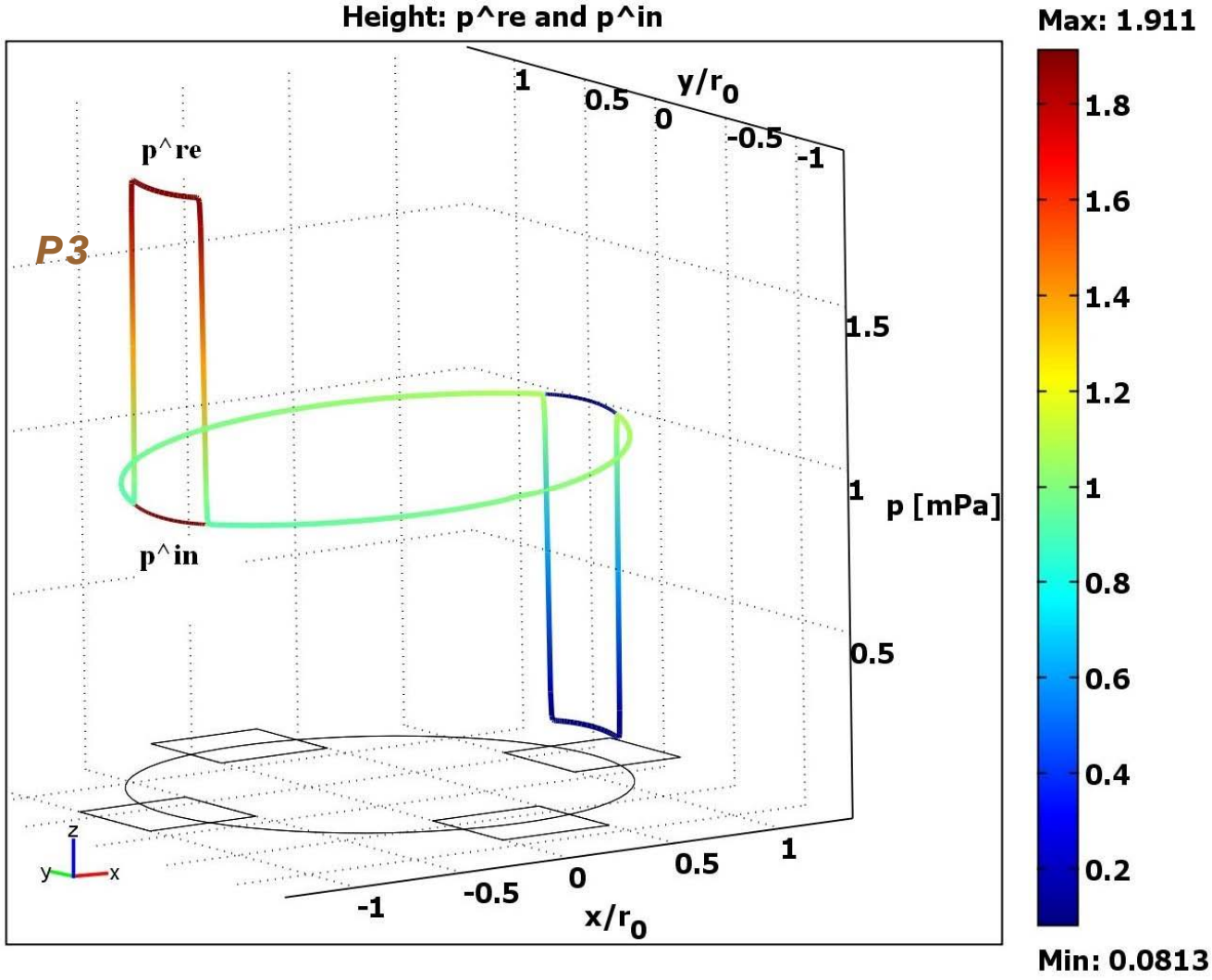
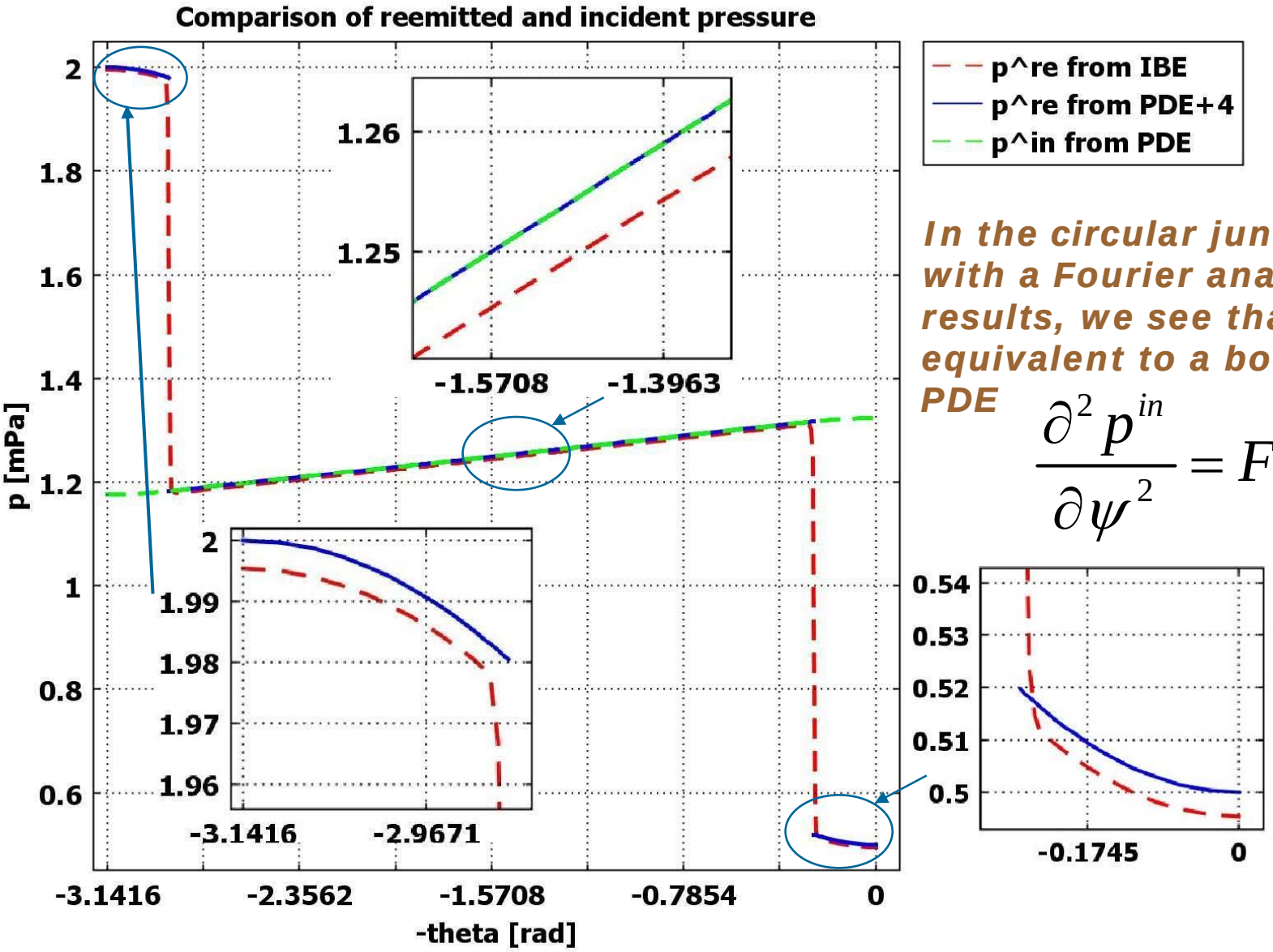


Fig 6: Elevation plot of simulation 'I' result for p^{re} and p^{in} with $p_0 = F^{ins}(P3) = 1$ mPa



In the circular junction, with a Fourier analysis of results, we see that IBE is equivalent to a boundary PDE

$$\frac{\partial^2 p^{in}}{\partial \psi^2} = F^{ins} \qquad (10)$$

Simulation 'II' results on wall for $-\pi < \psi < 0$; with details of input, middle and output regions, for IBE and for PDE eq 10, which is more precise (and exactly solvable)

4) RESULTS FOR THE SIMPLE OBSTRUCTION

It is convenient to fix p^{re} (instead of F^{ins}) at ports to reduce the number of dof and to see the effect of obstruction on the flow F^{ins} .

To see where $I_{AB}=0$ it is enough that one intersection with R2 is found (actually there are two). Moreover all points which belong to the same open segment are uncoupled because $\cos\vartheta_A=0$.

Convex corners $\beta<\pi$ requires more detailed considerations.

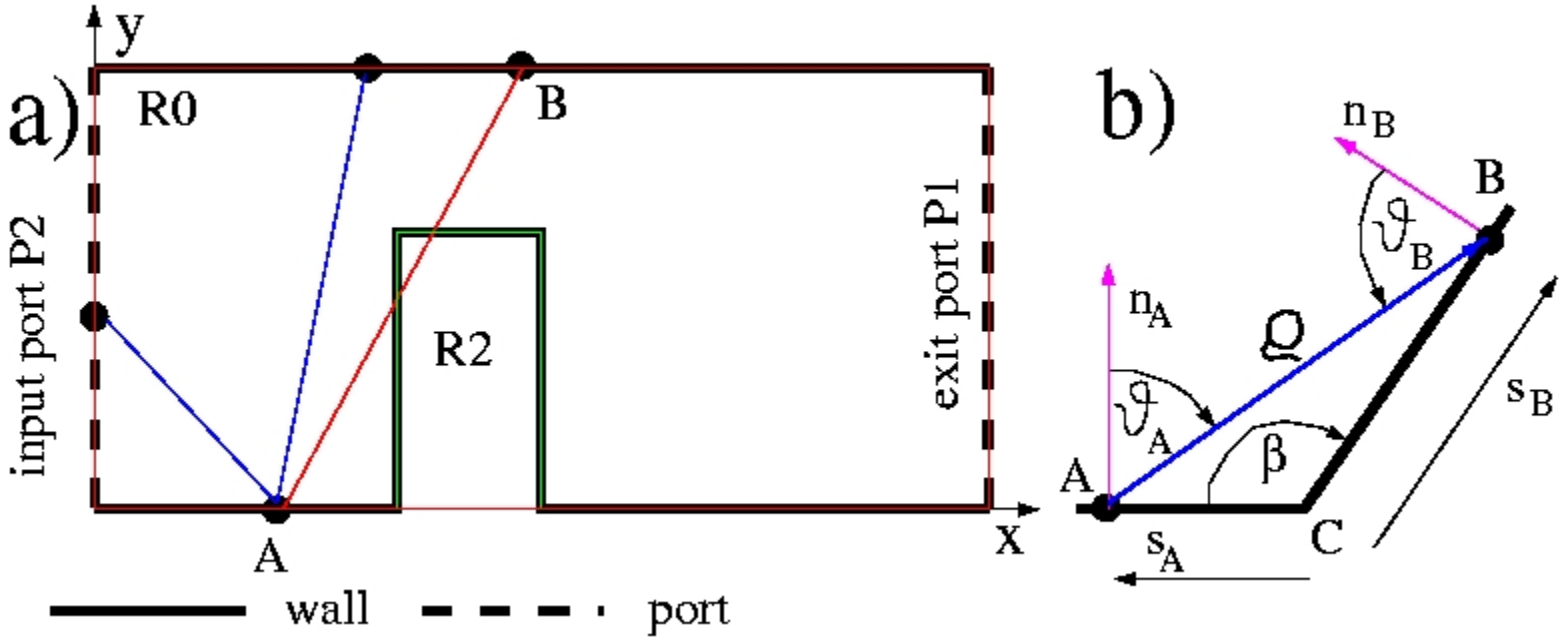


Fig 8: a) The simple obstruction, with a I_{AB} = 0 ray in red; b) a detail of a corner C

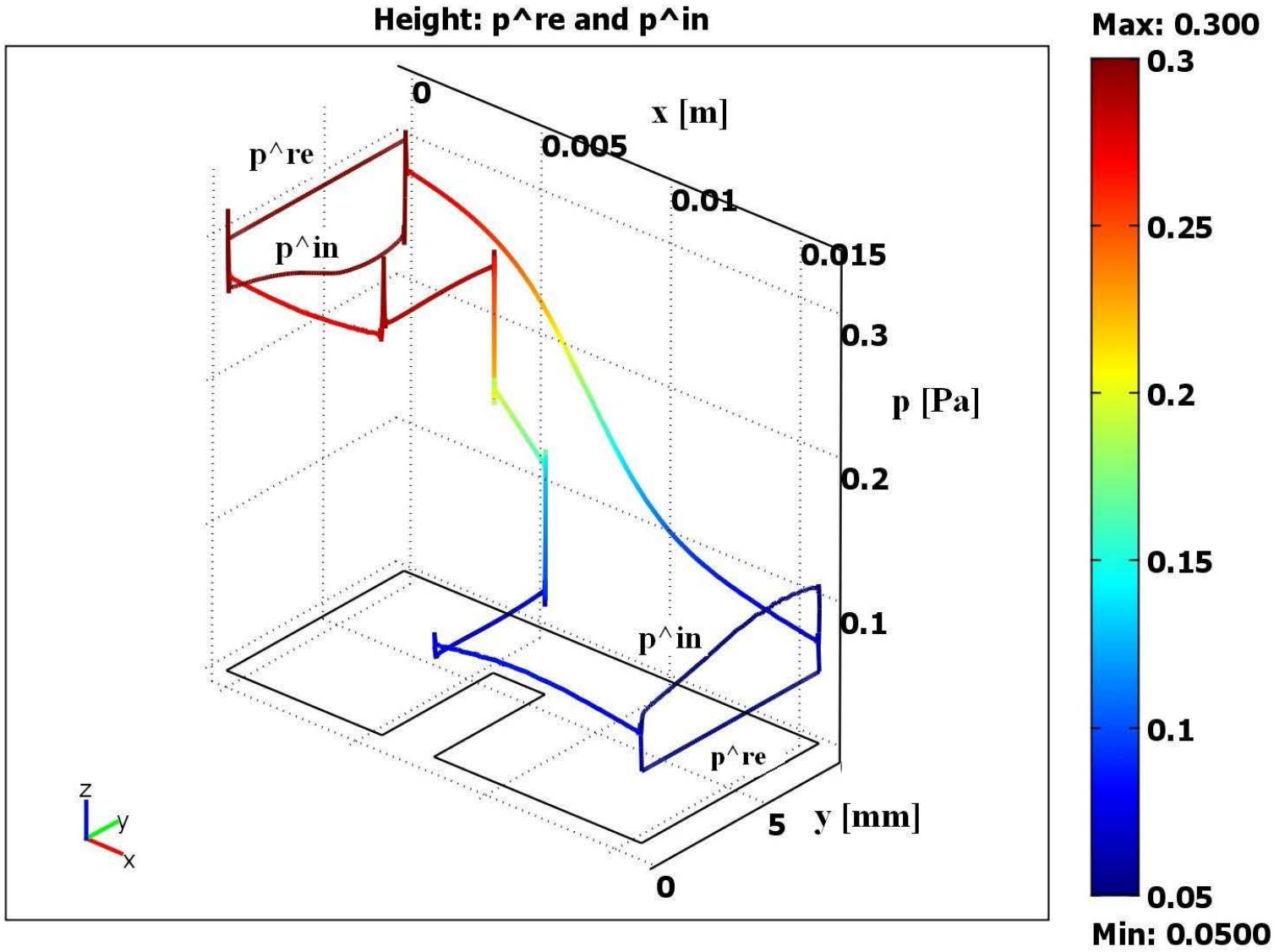


Fig 9: Elevation plot of simulation result for p^{re} and p^{in} with $p_2=0.3$ Pa and $p_1=50$ mPa. Spikes at some corners (see paper) do not significantly weight in the overall solution since ruling eq. is an integral equation)

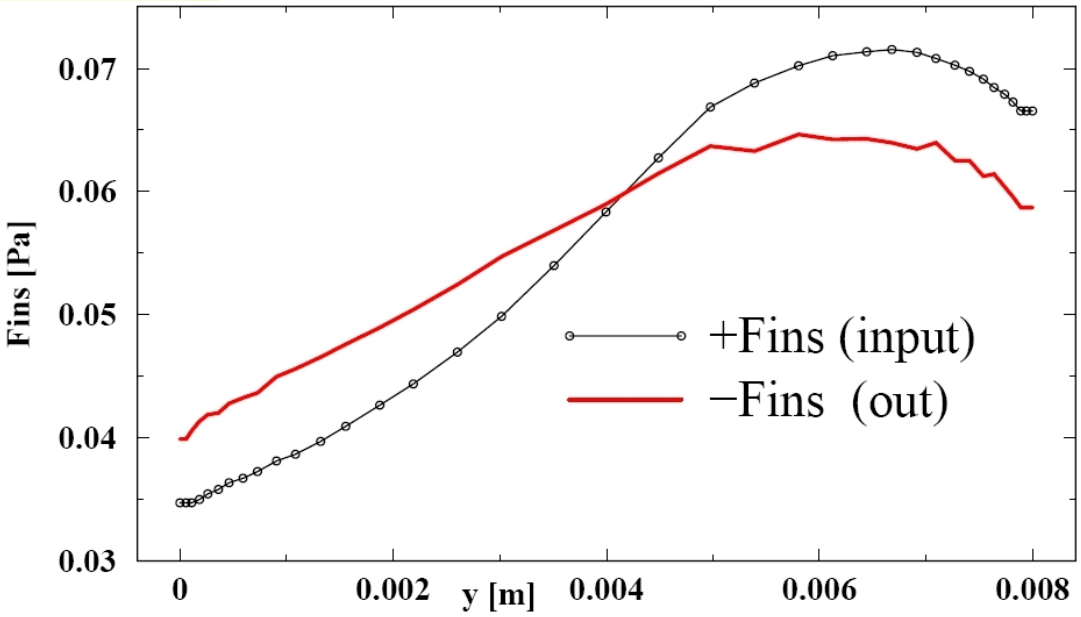
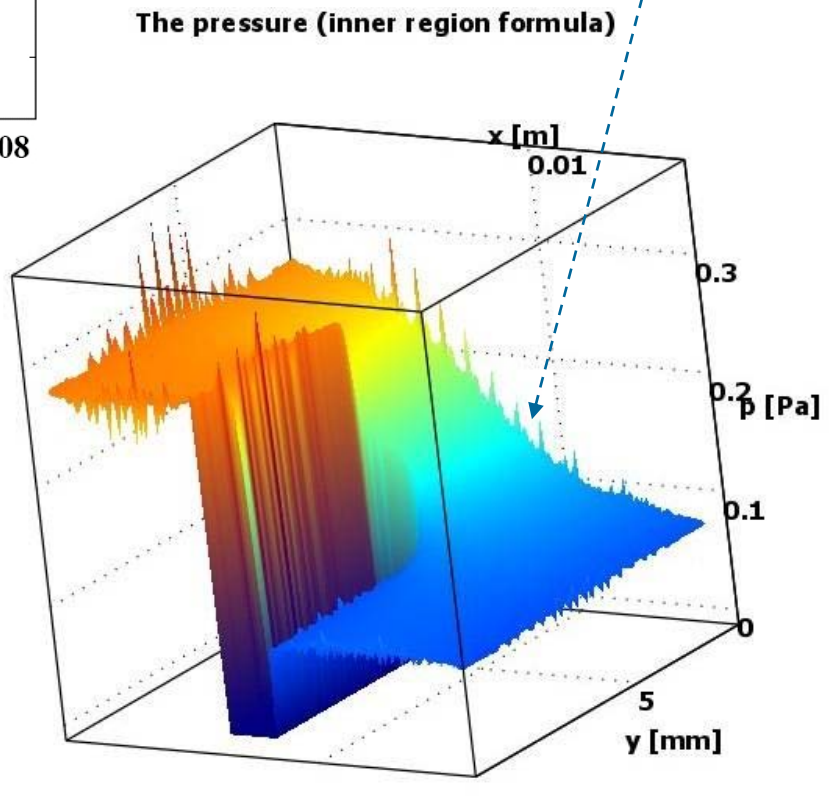


Fig 9: Input and exit flow density F^{ins} (here rescaled in Pa; to obtain the volumetric flow density F^{ins}, multiply by $v_{av}/4 = 120$ m / s for nitrogen at T=300 K); note that <u>net flow</u> is still non-uniform due the obstruction both at input and output

Fig 10: A surface plot of inner pressure pi: spikes near the boundaries are due to the $1/r_{AB}$ singularity, see eq 6



5) CONCLUSION

a) Gas pumping in molecular regime is isomorph to other very practical computational problems, as rendering the illumination in a room (computer graphics) or to thermal radiosity (high temperature ovens , beam targets, heat shields).

b) the boundary weak mode (with integral coupling) emerges as a natural solution method for molecular flow regime

c) in perspective, large vacuum devices may have regions where molecular flow applies and regions where compressible Navier Stokes eq. applies. Joining them seems a very useful task.

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See also:

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