Nitsche Method for non-Fourier Heat Conduction – Application and Limitations

Martin Sýkora

November 2024

1 Introduction

Heat conduction is often described by the Fourier law

$$\mathbf{q} = -k\nabla T,$$

which states that the heat flux $\mathbf{q}$ is proportional to the gradient of temperature T. The ratio is given by heat conductivity k. While this description is sufficient in many conditions, there are some settings, where a more detailed approach is needed, for instance heat conduction at very small size scales. A class of such approaches is called phonon hydrodynamics, see for instance [1, 2]. A new addition to the phonon hydrodynamics equations has been developed in [3]. This approach, derived from phonon kinetic theory through a first-order asymptotic expansion in the irreversible part and the Poisson projection in the reversible part, is rather complex. It incorporates both convection and diffusion, and therefore it highly resembles compressible Navier-Stokes equations. The equations read

$$\partial_t e = -\partial_i(c^2 m_i), \tag{1}$$

$$\begin{aligned}\partial_t m_i = &-\partial_i p - \partial_j\left(\frac{3c^2}{4e} m_i m_j\right) \\ &- \frac{1}{\tau_R} m_i + \frac{\tau c^2}{5}\partial_j\left(\partial_j m_i + \partial_i m_j - \frac{2}{3}\nabla\cdot\mathbf{m}\delta_{ij}\right)\end{aligned} \tag{2}$$

with pressure

$$p \approx \frac{e}{3} - \frac{c^2\mathbf{m}^2}{4e}. \tag{3}$$

Here, τ^{-1}, τ_R are relaxation times, c is the sound speed and the unknowns $e, \mathbf{m}$ stand for energy and phonon momentum. In [3], the authors performed numerical computations to demonstrate the effects the model can describe, like temperature drop past a cylindrical obstacle or von Kármán vortex street. The computations were non-physical (material parameters used for computations were nonrealistic) and they should be understood as theoretical experiments. However, even non-physical computations should not neglect the effects of boundary conditions (BCs). If one is interested in the behaviour of certain equations, they need to check, whether the result is dependent on the BCs used.[1] Therefore, the authors used both no-slip BCs, which are easy and straightforward to apply, and slip BCs applied by the so-called Nitsche method.[2] This method, however, containes a stabilisation parameter β, which was for siplicity ignored (i.e. set to zero) by the authors. In this text we show the effects of non-zero β and describe a potential risk when using Nitsche method.

2 Computations

2.1 Nitsche method

Wall boundary conditions assume there is no flux through the boundary, i.e. the normal component of momentum on boundary is zero:

$$\mathbf{m}_n = 0. \tag{4}$$

No-slip condition furthermore assumes that the tangential component of momentum $\mathbf{m}_\tau$ is zero as well. This means there is no motion at the boundary. On the other hand, the full-slip BC assumes the wall acts with no force in the tangential direction (there is no friction that would slow down the flow), or equivalently

$$(\mathbf{T}n)_\tau = 0,$$

where $\mathbf{T}$ stands for Cauchy stress and n for outer normal. These two BCs can be combined into the Navier-slip BC, which is given by

$$\Theta \mathbf{m}_\tau + \gamma(1-\Theta)(\mathbf{T}n)_\tau = 0. \tag{5}$$

Here, the parameter γ has the role of physical units (and we assume it is 1), while the parameter Θ describes to what extent is the wall slowing down the flow. Value $\Theta = 0$ leads to full-slip, while $\Theta = 1$ to no slip and values in between to partial slip.

As equations (1), (2) are similar to Navier-Stokes equations, the inspiration for the Nitsche method could be taken from [5, 6]. In [3] and [7], this is done by adding

$$\int \frac{\Theta}{\gamma(1-\Theta)} \mathbf{m}_\tau \cdot \mathbf{v}_\tau \mathrm{dS} - \int \left(\mathbf{T}(e,\mathbf{m})\mathbf{n}\right)_n \cdot \mathbf{v}_n \mathrm{dS} + \int \mathbf{m}_n \cdot \left(\tilde{\mathbf{T}}(f,\mathbf{v})\mathbf{n}\right)_n \mathrm{dS} \tag{6}$$

[1] For example the famous Poiseuille flow (parabolic velocity profile in a pressure-drop-driven flow in a straight channel) is *enforced* by no-slip BCs. For different BCs, the result, i.e. the velocity profile, could be completely different.

[2] Note, however, that there exist other approaches to BCs for phonon hydrodynamics; for instance the BCs presented in [4].

to the weak formulation of the equations (1), (2) with the unknown functions $e, \mathbf{m}$ and the test functions $f, \mathbf{v}$.[3] Here, $\mathbf{T}$ equals

$$\mathbf{T}(f, \mathbf{v}) = -\left(\frac{f}{3} - \frac{c^2\mathbf{v}^2}{4f}\right)\mathbf{I} + \frac{c^2\tau}{5}\left(\left(\nabla\mathbf{v} + \nabla\mathbf{v}^\top\right) - \frac{2}{3}\mathrm{div}(\mathbf{v})\mathbf{I}\right) \tag{7}$$

while $\tilde{\mathbf{T}}(f, \mathbf{v})$ is linearised.[4] In our case we do that by probably the simplest possible way – replacing some fo the occurances of $f, \mathbf{v}$ by solutions form the previous time step as

$$\tilde{\mathbf{T}}(f, \mathbf{v}) = -\left(\frac{f}{3} - \frac{c^2\mathbf{v}\cdot\mathbf{m}_0}{4e_0}\right)\mathbf{I} + \frac{c^2\tau}{5}\left(\left(\nabla\mathbf{v} + \nabla\mathbf{v}^\top\right) - \frac{2}{3}\mathrm{div}(\mathbf{v})\mathbf{I}\right), \tag{8}$$

but a more sophisticated implementations can be used, for instance by using UFL derivative. In this text we add stabilisation term

$$\frac{\beta\tau c^2}{5h}\int \mathbf{m}\cdot\mathbf{v}\mathrm{dS}, \tag{9}$$

where h is the minimum edge length and β is a parameter to be set. This term is optional for non-symmetric Nitsche and necessary for symmetric Nitsche, see [8].

2.2 Setting and results

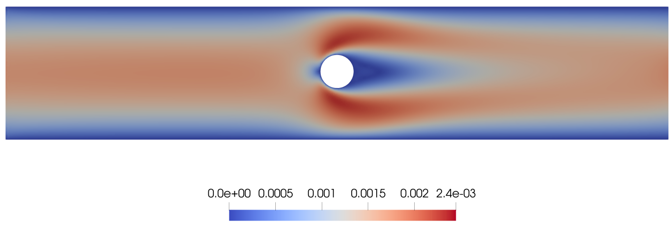
The overall setting is shown in Figure 1a. We have a straight channel with a cylindrical obstacle. The phonons are moving from left to right. In order to compare different results, we plot the momentum over a vertical line just right to the cylindrical obstacle. We use a reference mesh of approximately 47000 cells and its refinements aroung the cylinder. This mesh and the vertical line are shown in Figure 1b. The exact material and geometry parameters are specified in the codes accessible here.

Let us compute the momentum flow through the cylinder boundary[5] for different β over the two meshes, compared to the inlet flow. We compute the flux over the reference mesh and its level-six local refinement around the cylinder. Each refinement roughly shortens the edge length twice, so the finer mesh has 64 times shorter edges on the cylinder. The result is summarised in Figure 2. One can see that with increasing β, the flux through cylinder wall decreases, especially for the rougher mesh. Higher β can lead to higher computational requirements, but in this simple setting the differences are negligible. In the following paragraphs, we compare the original choice $\beta = 0$ from [3] with $\beta = 10000$, which gives the smallest flux through the cylinder boundary.

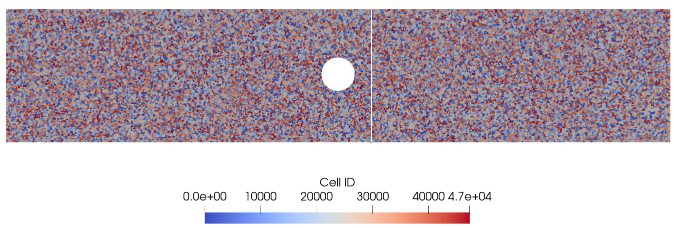
[3] We are using non-symmetric Nitsche method. If the signs before the second and third term in (6) are both minuses, the method is called symmetric Nitsche.

[4] We want to be testing by linear expressions of our test functions.

[5] We want it to be as close to zero as possible so that the impermeability condition (4) is valid.



(a) Phonon momentum in a flow past a cylinder.



(b) Reference mesh used for most computations and a line over which we plot the velocities.

Figure 1: The geometry of the problem.

2.2.1 Case $\beta = 0$

As the BC is not exact (see the large flux through cylinder wall), we need to refine the mesh a lot, at least around the cylinder, until the solutions converge. Figure 3 shows the flow over the highlited cross-section for various levels of refinement. We can see a reasonable level of convergence at around levels 6 or 8. Therefore one needs to decrease the edge length roughly 2^7 times to reach the convergence.

2.2.2 Case $\beta = 10000$

We perform the same test with level zero, one and two refinement. The result is shown in Figure 4. The solutions are nearly the same, so the convergence seems to be reached without any refinement. However, the result are different from the graphs in Figure 3, so at least one of them needs to be wrong. Moreover, Figure 1a shows the flow with $\beta = 10000$ and no refinement. Note the near-zero momentum around the cylinder, which suggests no-slip condition. To understand this, we need to perform even more refinements as in Figure 5. The figure also shows the result with Dirichlet no-slip BC on the cylinder (with

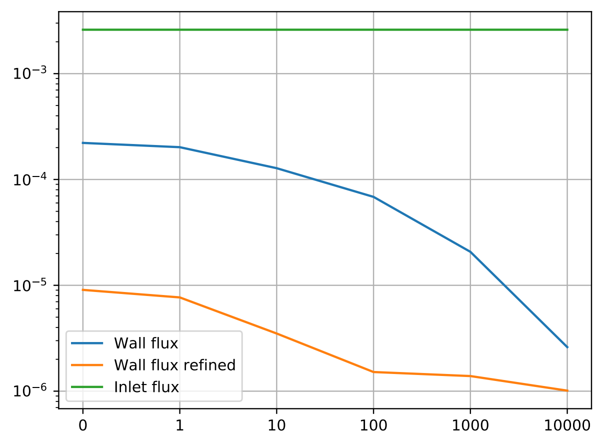


Figure 2: Flux through the cylinder wall on the reference mesh (blue line) and refined mesh (orange line) and the inlet flow (green line). With increasing β, the flux through wall decreases.

no refinement). As we can see, the results with no to two refinements closely resemble no-slip BC instead of full slip and show a seeming convergence, then a transitional phase between no-slip and full-slip is observable and at around refinement level twelve the method converges. Such refined mesh – even though locally – needs millions of elements, which is far beyond real applicability. The finest solution is plotted in Figure 6 – unlike Figure 1a we can see slipping at the cylinder.

2.2.3 Optimal β

Performing the same test for $\beta = 10, 100, 1000$ we search for optimal value ensuring the fastest convergence. The results are shown in Figure 7. The best value seems to be around 100 with no major difference between the symmetric and non-symmetric variants.[6] However, even with the best choice one still needs to perform at least four refinements, which is too much for real applicability.

2.2.4 Everything is lost. Right?

No, not really. Indeed, the mesh size needed for convergence is too small for realistic applicability, especially in 3D computations. However a few comments should be made here. First, not all possibilities were tried, especially symmetric Nitsche method, but also other valoues of β, for instance between 10 and 100.

[6] A more proper comparison of symmetric and non-symmetric Nitsche should be performed to draw proper results.

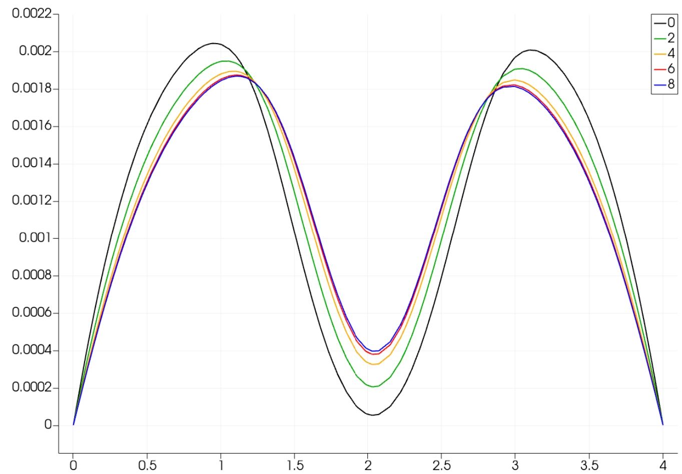


Figure 3: Phonon momentum past a cylindrical obstacle with $\beta = 0$ for various levels of mesh refinement. Higher level means finer mesh.

Maybe one could fine a little better results with them. Second, the results are dependent on the software used (here FEniCS 2019.1.0) and implementation of the algorithm. For instance different ways to measure the minimum edge length or normal vectors might change the speed of convergence. The topic of normals was studied in [5]. The work compare three types of normals. The first, analytic, can only be used in geometries, where the normal could be computed analytically, and it gives by far the best result. It would probably speed our convergence, since the normal to the cylinder/circle is known, but it cannot be used in a general case. Then the authors compare two other normals called facet normal (used by us as well) and vertex normal. Each of them has its benefits, but especially for symmetric Nitsche the vertex normal might be advantageous. Since symmetric Nitsche seems to be working well, see Figure 7, using symmetric Nitsche with vertex normal might lead to significantly better results. Another big question is the way to linearise the Cauchy stress. The author of this text tried another variant – taking derivative of $\mathbf{T}(e, \mathbf{m})$ with respect to the variables $(e, \mathbf{m})$, using UFL derivative, and multiplying by the test functions $(f, \mathbf{v})$. This gives a linear (in test functions) approximation of the stress, but the result were comparable to the use of $\tilde{\mathbf{T}}$, but again a more proper testing would be needed to draw decisive conclusions.

To conclude, trying symmetric Nitsche with vertex normal and various values of β would probably lead to somewhat better convergence in this specific case. That beeing said, the non-symmetric Nitsche has unsatisfactory performance only in this very setting – the relaxation times, sound speed, geometry etc. Actually, we can perform the very same computations with Dirichlet no-slip on the cylinder and full-slip on the walls. Since the walls are straight and aligned with the x-axis, the full-slip BC on them can be prescribed in the Dirichlet sence

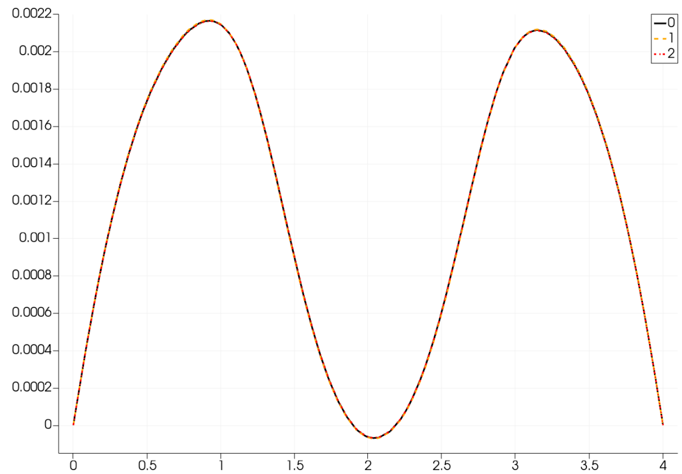


Figure 4: Phonon momentum past a cylindrical obstacle with $\beta = 10000$ for various levels of mesh refinement, black = level zero, orange dashed = level one, red dash dotted = level two. Since the three results are nearly undistinguishable, a seeming convergence is reached.

as well. The comparison of the result is shown in Figure 8 – one is Dirichlet full-slip BC and the other non-symmetric Nitsche with $\beta = 10000$ and no refinement. Even though this value of β performed poorly on the cylinder, it gives perfect results on the walls. Since full-slip is often used on the walls and not on a obstacle in the middle of the flow, for instance in blood flow modelling, Nitsche method is far from useless. The reason why there is such a tremendous difference in performance of Nitsche method between walls and cylinder is unknown up to our knowledge. Some of the principal differences are that the boundary of the cylinder is curved and is exposed to much stronger flow than the walls, which are essentially tangential to the flow.

2.2.5 Navier-Stokes equations

One might suggest that Nitsche method gives different results for different equations and that its behaviour is better known for Navier-Stokes equations then for phonon hydrodynamics. Our results might be coused by the fact that we are applying Nitsche method to equations which are not understood properly. However, this is not the case. It is possible to reach similar results for incompressible Navier-Stokes equations as well. We perform a similar computations with non-symmetric Nitsche[7] with $\beta = 1000.$ on a slightly changed geometry – the channel has dimensions 2.2×0.41, the cylinder has radius 0.05 and centre at $(1.1, 0.2)$. The fluid has density $\rho = 1000$, kinematic viscosity $\nu = 0.005$ and the

[7]The method is the same, but as the stress is linear for Newtonian fluids, we do not need to linearise it.

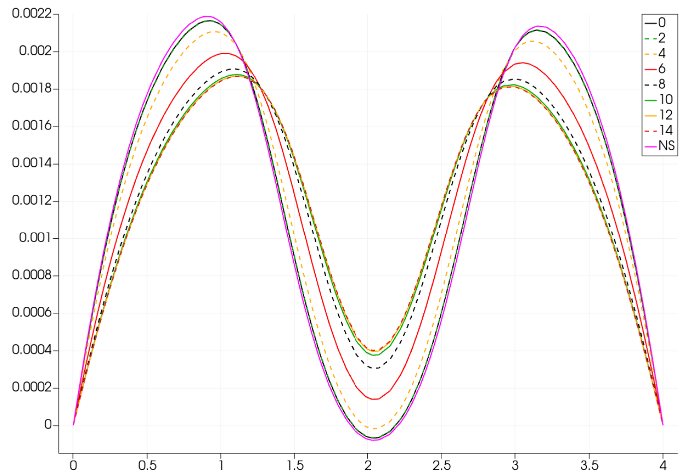


Figure 5: Phonon momentum past a cylindrical obstacle with $\beta = 10000$ for various levels of mesh refinement compared to no-slip BC on the cylinder. For not enough refinement, the solution is closer to the no slip BC than to the actual full slip. The seeming convergence for levels zero to two is not real.

inflow is given as $(\frac{6}{0.41^2}y(0.41-y), 0)$ and the reference mesh has approximately 44000 elements.

We perform computations on different levels of refinement, see Figure 9, and obtain similar speed of convergence to phonon hydrodynamics (compare to Figure 7).

3 Conclusion

In this text, we optimised the choice of stabilisation parameter β for non-symmetric Nitsche method used to enforce full slip on a cylinder in a flow of phonons. This choice speeds-up the convergence in comparison with the trivial choice $\beta = 0$, although still being very slow and probably not usable in 3D computations. If simple geometry is used, using the analytic normal might give better results. If the analytic normal is not known, we suggest trying the vertex normal and symmetric Nitsche method. They may give slightly better results.

The unsatisfactory results lead us to the second topic of this text, and that is a warning about the method. The results can be summarised as follows:

- Increasing β leads to decreasing flux through boundary.
- This lower flux, however, does not guarantee a better convergence rate.
- Each β seems to be linked with two values max_β and min_β. For mesh size greater than max_β, Nitsche method enforces no-slip-like BC (even

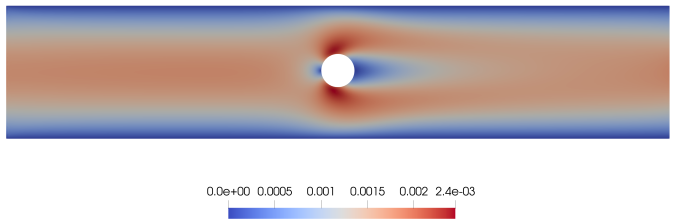


Figure 6: Phonon momentum past a cylindrical obstacle with $\beta = 10000$ and level fourteen refinement. One can observe expected slip behaviour at the cylinder, unlike the non-refined solution in Figure 1a.

though the slipping parameter Θ is equal to zero, which means a full-slip). For mesh size smaller then min_β, Nitsche method enforces full-slip nearly perfectly and for values in between there is a transitional phase between the two.

- Consequently, on rough meshes a seeming convergence might happen with the no-slip-like BC.
- Values of min_β, but also max_β could be so small that meshes commonly used in computational fluid dynamics are too rough and fall into the no-slip-like zone.
- Values of min_β and max_β might decrease with increasing β, meaning a finer mesh is needed. This happens for too large β, which further explains the second point.

As for possible future work, it might be suggested to study the possibilities mentioned above (different normals, symmetric Nitsche etc.). Moreover, this text only measures flux through boundary and shows convergence on figures. It would be appropriate to also include more exact measures of convergence; for instance integral norms.

Finally, let us describe once again the theoretical danger of Nitsche method. A CFD expert tests non-symmetric Nitsche method with $\beta = 10000$ on the straight walls and compares the result with Dirichlet full-slip. The result on the reference mesh is the same, see Figure 8, so they use it on the cylinder (with no slip on the walls). They perform computations on three meshes with roughly 12, 27 and 47 thousands elements (the finest is the reference mesh) and get results shown in Figure 10. As mesh refinement does not change the result, they conclude that the true solution has been reached, even though we already know that this is just the seeming convergence. Good behaviour of Nitsche method at one boundary part does not imply that it will give good results on another boundary part. When we see convergence, we need to check, whether

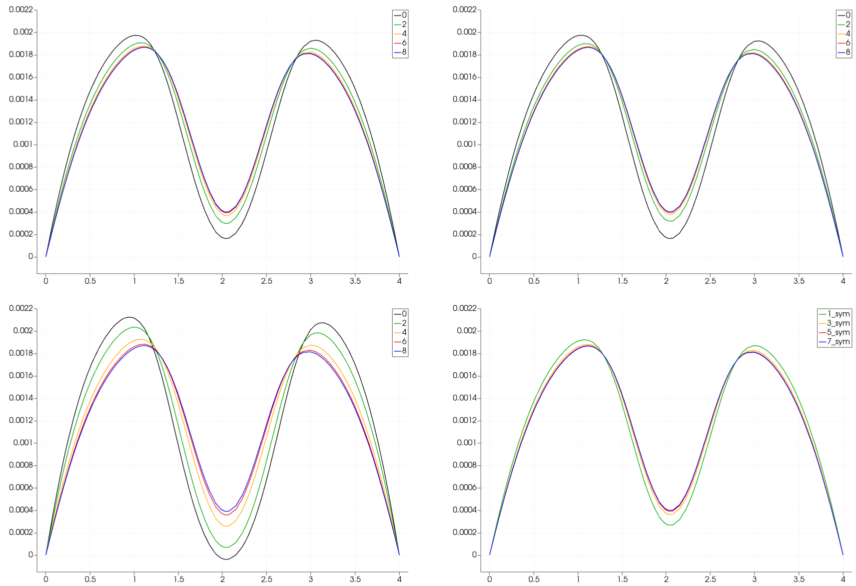


Figure 7: Phonon momentum past a cylindrical obstacle with various values of β and mesh refinement. Top left = ($\beta = 10$), top right = ($\beta = 100$), bottom left = ($\beta = 1000$), bottom right = ($\beta = 100$) and symmetric Nitsche is used. Out of non-symmetric variants, 10 and 100 are close, 100 performing slightly better. Both are better then ($\beta = 0$). Value 1000 perform by far the worst, but still better then value 10000 from previous section. The symmetric variant needs one refinement less to reach similar results as value 10 non-symmetric Nitsche.

there is some non-trivial slip on the boundary. If not, it might be the seeming convergence.

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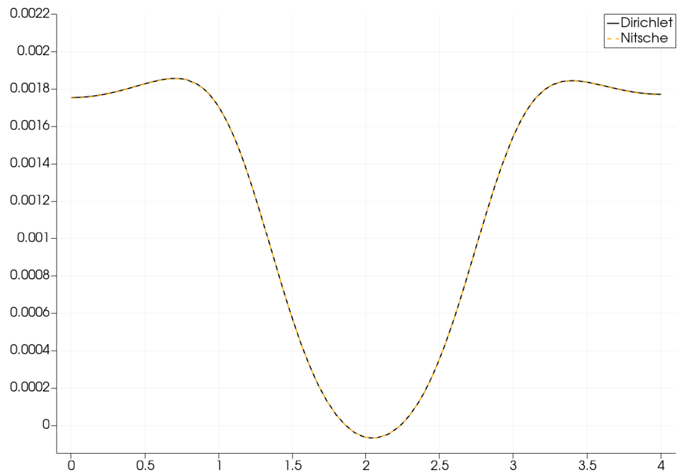

Figure 8: Phonon momentum past a cylindrical obstacle with no-slip BC on the cylinder and full-slip BC on the walls. Dirichlet and Nitsche method with $\beta = 10000$ give the same result.

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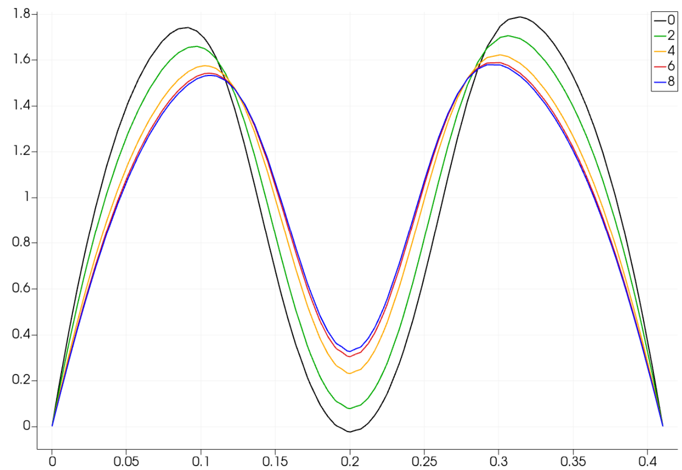

Figure 9: Flow of newtonian fluid around cylinder. Velocity profile behind the cylinder for $\beta = 1000$ for various levels of mesh refinement. The speed of convergence is nearly identical to that of phonon hydrodynamics with the same β, see Figure 7.

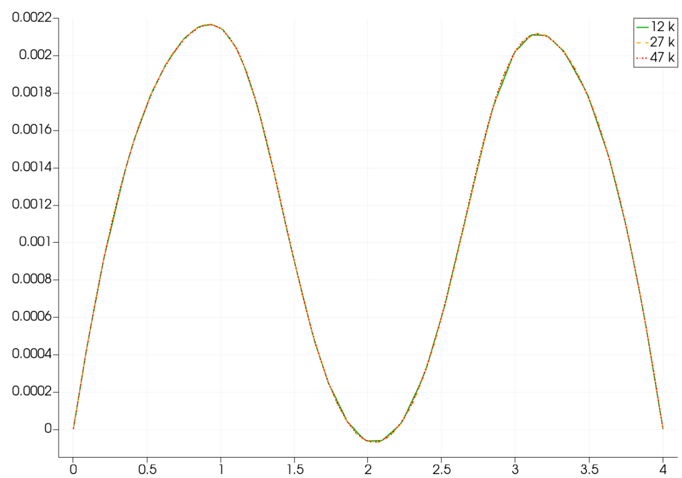

Figure 10: Phonon momentum past a cylindrical obstacle with $\beta = 10000$ for meshes with roughly 12 k elements (green line), 27 k elements (orange dashed line) and 47 k elements (red dash dotted line).