**Theory Manual for CaNS 2.0**

This document explains the numeric in CaNS 2.0. The solver uses the projection method on staggered grids.

**1. Staggered grid**

We show the calculation of convective and viscous terms on a staggered grid,



The following scheme can be derived via finite difference/volume. Here, we regard it as a finite volume scheme. Taking 2D problems as an example, the two terms in the direction,





The two terms in the direction.





In the projection method, we also need the divergence of velocity and the gradient of





Figure 1 shows the stencils for solving , and .



Figure 1 Stencil points for solving , and

We assume a discontinuity between the wall and the first off-wall location. Across the discontinuity,  is large, while ,  and  are not large. Consequently, we should avoid the interpolation (reconstruction) or the differencing operator , where  is 1, or . Instead, one-sided operation biased towards the domain should be adopted. Table 1 lists the relevant terms in Eq. -. The conclusion is that no special treatments are needed near the wall for the projection method on a staggered grid,

Table 1 Terms that contain  or  in Eq. -

|  |  |  |
| --- | --- | --- |
| Eq. | Related term | Explanation |
|  |  | due to  on the wall |
|  |  | , computed from wall model |
| - | No |  |

A hand holding a piece of paper

Description automatically generated

I think there are basically two mistakes in the solution.

(1) Both velocity and its gradient are used at the wall, which makes the problem ill-posed (overdetermined). We should use only the velocity gradient as the wall boundary condition in WMLES; the velocity at the wall is non-zero.

(2) We should avoid differencing operator  across the layer between the wall and the first off-wall point. As Larsson reminded, that layer is under-resolved (discontinuous) in WMLES, so the wall-normal derivative computed using the wall point and the first off-wall point is incorrect. However, this solution does an interpolation using the velocity values at positions 1 and 2 and the velocity gradient at the wall, which implies that it assumes a smooth profile of velocity from the wall to position 1 to position 2. The assumption does not hold true, so this treatment can cause large errors.

In contrast, I still believe my current implementation is correct. It guarantees that the term  in Eq. . As for using ghost cells, it is just for convenience to guarantee , and for consistency with CaNS using ghost points for all kinds of boundary conditions. The size of the ghost cells is not important, as long as  can be exactly yielded. In CaNS, the ghost cells have the same size as the first off-wall cells , and . This exactly yields . As for , it is just normally computed as , using only the velocity information at positions 1 and 2.

Figure 2 shows the wall gradients provided by a wall model. In essence, only four locations need to be assigned values by the wall model, which uses, as input, the information at four interior locations.



Figure 2 Gradients provided by a wall model

Figure 3 shows a splitting of the domain into two subdomains. The calculation of wall gradients by the wall model only uses, as input, the information at interior points. Hence, it is confirmed that wall model is allowed to be called before updating ghost cell information.



Figure 3 Splitting of domain

**2. Poisson equation solver**

The elliptic Poisson equation is



It can be solved via iterative methods, like Jacobi, Gauss-Seidel (with successive overrelaxation). ADI can be used, but it also needs iterations for a second-order accuracy in unsteady flows. This is different from AF method, whereby no iteration is involved if accurate  and  in  (assuming  is a constant matrix). However, there is no factorization of Poission equation. Fourier transform can be exploited for obtaining tridiagonal matrices. For a 3D problem with two periodic (homogeneous) directions, namely and , and one non-homogeneous direction, , it requires two consecutive FFTs in the homogeneous directions. In the following,  and ;  and  denote the number of cells,



Fourier series in the direction,



Fourier series in the direction,



Hence,



Inserting Eq. into Eq. ,



A modified wavenumber is defined as





Strictly speaking, the definition of eigenvalue  includes , but it is left out here for consistency with Costa’s article. Inserting Eq. into Eq. ,



For a given set of , Eq. is a tridiagonal system of equations; there are in total systems of equations. If uniform grid spacing in the direction,



This also required a uniform grid spacing in the z direction, which might be the reason that Eq. is the set of equations solved in channel flow. In addition, it is more efficient to solve a tridiagonal system of equations than a third Fourier transform. For a square duct with homogeneous Neumann boundaries in the direction, IDCT-II is performed in that direction. Please refer to Numerical Recipes for the relationship between DFT and DCT. On a staggered grid where is stored at the cell centers from 0 to , Eq. and Eq. provide the formulations of DCT-II and IDCT-II. Performing cosine series expansion of in the direction after Fourier series in the direction (Eq. ),



Inserting Eq. into Eq. ,



Modified wavenumber is defined as





Hence,



It has the same form as Eq. , which includes equations. Note that the wavenumber *kx* is always indexed as 0,1,…,, with the number of those input points, even if the input data points are indexed as 1,2,…,*N*. For example, the input data points are indexed as *i*=1,2,…,*Nx* in CaNS, then *kx* is *i*-1.

The kind of transform is determined by the boundary conditions of , nothing to do with *R*, because the ghost cell values of *R* are not used in either the physical space or the spectral space, whereas the ghost cell values of are used in both spaces. In contrast, the ghost cell values of is used. In the following, we denote the form of Eq. and as



Hence, we need to solve



For nonuniform grid spacings in the z directions,



That is,









Now, we consider the boundary conditions. In this regard, special care should be given to the calculation of  in the right hand side and *b* in the left hand side.

For Poisson equation, the right hand side of Eq. in internal cells is



For boundary cells, the calculation of  has to consider the boundary conditions in the implicit directions. For Poisson equation, thee directions need to be considered, and for momentum equations, three directions or only z directions need to be considered. Here, we take z direction as an example to illustrate its calculation. The Poisson equation at pressure cell (*i*, *j* ,*k*=1) is



If Dirichlet boundary condition,



Here, the boundary condition can be homogeneous (*c*=0) or nonhomogeneous (c≠0) in this step. If we assume periodic boundary conditions in the *x* and *y* directions,



That is,







In the following, we list the calculation of *b* and  for various boundary conditions.

If Dirichlet boundary conditions,







If Neumann boundary condition,







If periodic boundary conditions,







Eq. can be solved using Thomas algorithm for periodic tridiagonal systems. We would like to highlight that the calculation of  for boundary cells do not require homogeneous boundary conditions, whereas the Fourier transform requires homogeneous boundary conditions.

For a modified Poisson equation,



where is a known function of the coordinates,



**3. Low-storage Runge-Kutta scheme**

We use symbols in Orlandi’s book. In CaNS, the low-storage Runge-Kutta scheme is combined with the projection method (Harlow and Welch, 1965; Chorin, 1968; Kim and Moin, 1985)









where,  and . The variable  is not needed due to . The operator  denotes nonlinear terms, including convective term and modelled stress term,



where is modelled stress. The operator  is second-order derivative. The coefficients



The stability condition is



Its implementation is



The eddy viscosity part is typically much less than the viscous part, so it can be neglected. As the Reynolds number increases, the inviscid part dominates the stability condition. If the viscous term is treated implicitly in all the three directions,



Let ,



The right-hand side of Eq. is similar to that of Eq. . Let ,



Expand it,



If  is discretized via second-order central differencing, the left-hand side of Eq. is a heptadiagonal matrix. In 2D problems, it is a pentadiagonal matrix (see Apeendix A). The modified Helmholtz equation Eq. can be solved via approximate factorization (AF) or transform method.

If the viscous term is treated implicitly only in the direction,



Let ,



Let ,



Expand it,



The left-hand side of Eq. is a tridiagonal matrix. Compare the RHS of Eq. , and ,



In a computer code, the explicitly treated terms are lumped/stored together, and the implicit terms are stored together. In CaNS, the implementation of Eq. and is



The solved variable is  directly, rather than .

In LES, eddy viscosity is introduced. Consequently, the hybrid RK-CN scheme Eq. becomes



where operator  denotes the viscous term,



Re-express it using ,



Let ,



Expand it,









Eq. is no longer a modified Helmholtz, so transform method cannot be applied. If we simplify the viscous term as did in Bae’s code, Eq. becomes





**4. Approximate factorization**

Equation with 3D implicit viscous diffusion can be solved via approximate factorization. Introducing matrix symbols (not tensors) ,  and ,



Note that each of ,  and  is a tridiagonal matrix. Using approximate factorization (AF),



Re-expressed as



The sweep procedure is described in Anderson’s book (P245). In the *i* direction,  is first solved, then , etc. In summary, hybrid Runge-Kutta/Crank-Nicolson finally solves tridiagonal systems of equations, and there are no constraints on the kinds of boundary conditions. The three-step explicit Runge-Kutta helps improve the accuracy, and the implicit Crank-Nicolson helps increase .

**5. Transform method**

Equation with 3D implicit viscous diffusion can be solved via transform method,



The formulations of the eigenvalues are given in Table 6 and Table 7 in Appendix C. Note that both staggered and non-staggered transforms are used. In a square duct, and use staggered and non-staggered transforms in the direction, respectively.

In CaNS, transform method (non-staggered) is also used in the and direction when the diffusion term is treated implicitly in all the directions. Table 2 lists the theoretical limitations of CaNS, and Table 3 lists the actual limitations. The same constraints apply to both the implicit and implicit 1D scheme. Consequently, the wall modeling capability always applies in the direction, and only in explicit (or implicit 1D) form, applies to and directions. Also note that homogenous Neumann boundary condition always applies for walls with/without wall models, due to the no-penetration wall-normal boundary condition.

Table 2 Limitations of time-advancement schemes

|  |  |  |  |
| --- | --- | --- | --- |
|  | Explicit RK | Hybrid RK/CN | Hybrid RK/CN (1D, *z*) |
| Mesh- | Uniform | Uniform | Uniform |
| Mesh- | Uniform | Uniform | Uniform |
| Mesh- | Non-uniform | Non-uniform | Non-uniform |
| cbcvel- | PP, DD, NN, DN | PP, D0D0, N0N0, D0N0 | PP, DD, NN, DN |
| cbcvel- | PP, DD, NN, DN | PP, D0D0, N0N0, D0N0 | PP, DD, NN, DN |
| cbcvel- | PP, DD, NN, DN | PP, DD, NN, DN | PP, DD, NN, DN |

Table 3 Limitations of CaNS

|  |  |  |  |
| --- | --- | --- | --- |
|  | Explicit RK | Hybrid RK/CN | Hybrid RK/CN (1D, z) |
| Mesh- | Uniform | Uniform | Uniform |
| Mesh- | Uniform | Uniform | Uniform |
| Mesh- | Non-uniform | Non-uniform | Non-uniform |
| bcvel- | PP, DD, NN, DN | PP, D0D0 | PP, DD, NN, DN (PP, D0D0) |
| bcvel- | PP, DD, NN, DN | PP, D0D0 | PP, DD, NN, DN (PP, D0D0) |
| bcvel- | PP, DD, NN, DN | PP, DD, NN, DN | PP, DD, NN, DN |

**6. LES**

The nondimensionalized log law reads as



We use Newton-Raphson to solve in Eq. . We construct





The Newton-Raphson iteration formula is



The current coupling is though modifying the ghost cell wall-parallel velocity values to match the wall stress yielded from a wall model. No-penetration boundary condition is applied on the walls, so zero convective flux is guaranteed; this implementation strategy ensures no convective flux on the walls. Of course, there is slip velocity on the wall. For a general velocity profile,





We have









Note that







For brevity, we do not include viscosity. At the wall, , and , so















In equilibrium wall models, we assume that the velocity direction does not vary with *y* within the wall model layer, i.e., . Consequently,















Eq. - are the same as Eq. -, but note that  is different from  in 3D TBLs. Hence, one possible strategy of wall modeling for 3D TBL is to predict the magnitude of wall shear stress and its direction, respectively. In the current log-law wall model,  is assumed, that is, the direction of velocity does not vary in the wall model layer, while its magnitude varies as a classical near-wall law.

The classical Smagorinsky model read as



where , and van Driest damping function



For varying eddy viscosity, the viscous term becomes







where the stress tensor , with the isotropic part ignored in the Boussinesq assumption. It can also be expressed as







The resolved viscous terms can be treated either explicitly or implicitly, whereas the modelled terms, like the inviscid terms, are always treated explicitly. It is convenient to lump the modelled terms together with the inviscid terms. Consequently, we only need to add the modelled terms to the right hand side even if the viscous terms are treated implicitly. In contrast, if a wall model is used to change the boundary conditions and an implicit scheme is used, we have to further modify the right hand side at boundary cells to reflect the change of boundary condition values, assuming that a Neumann boundary condition is already set. When adding a wall model, we do not need to consider that homogeneous boundary conditions must be used in the FT direction, because the modification to the right hand side is irrelevant to FT. Before FT, all aspects have been considered in the physical space. We just need to be aware that the resulting wall model should not be used in the FT directions. Due to the added eddy viscosity, the time step criterion has to be altered. Specifically, variable  should be added to Eq. . However, this may not be important when the viscous term is treated implicitly, though it may be necessary when the viscous term is treated explicitly.

**7. Verification and validation**

Verification is to demonstrate that a wall model has been correctly implemented into CaNS. It is done via comparison to other codes or analytical solutions (if existing). Validation is to demonstrate whether a model is good or not, in terms of representing/modeling the true physics. It is done via comparing to experiments, or analytical solutions (if existing). Here, verification is needed to show if the implementation of wall model is correct.

Table 4 Selected verification cases

|  |  |  |
| --- | --- | --- |
|  |  | Time advancement |
| Laminar channel2D |  | Explicit |
| Laminar channel2D |  | Implicit 1D |
| Laminar channel3D |  | Explicit |
| Laminar channel3D |  | Implicit 1D |
| Turbulent channel2D | 180-10^10 | Explicit |
| Turbulent channel2D | 180-10^10 | Implicit 1D |
| Turbulentchannel3D | 180-10^10 | Explicit |
| Turbulent channel3D | 180-10^10 | Implicit 1D |

Table 5 Selected validation cases

|  |  |  |
| --- | --- | --- |
|  | Re | Time advancement |
| Square duct |  | Explicit |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |

**Appendix A**

For an interior , and control volumes, we have





In the following, we derive the Poisson equation of pressure. We define



We have



where



We should have  for every cell at the end of the time cycle. Hence,





Eq. , , , are the set of equations used for solving the Navier-Stokes equations. When there is variable eddy viscosity, the viscous term is





**Appendix B**

The seven-diagonal systems of equations from Eq. is



Pentadiagonal matrix yielded from Eq. in 2D problems.



**Appendix C**

The eigenvalues are given by . Table 6 and Table 7 list the transforms and inverse transforms for different combinations of boundary conditions. is the number of input points, 0,1,…,, instead of the number of cells. Zero-value points are always left out. The current index of input points is consistent with scipy and wiki. The factors in the inverse transforms are consistent with Costa’s paper and scipy.

Table 6 Transforms on a staggered grid

|  |  |  |  |
| --- | --- | --- | --- |
| BC |  | Transform | Inverse transform |
| PP |  | DFT | IDFT |
| NN |  | DCT-II | DCT-III |
| DD |  | DST-II | DST-III |
| ND |  | DCT-IV | DCT-IV |
| DN |  | DST-IV | DST-IV |

Table 7 Transforms on a non-staggered grid

|  |  |  |  |
| --- | --- | --- | --- |
| BC |  | Transform | Inverse transform |
| PP |  | DFT | IDFT |
| NN |  | DCT-I | DCT-I |
| DD |  | DST-I | DST-I |
| ND |  | DCT-III | DCT-II |
| DN |  | DST-III | DST-II |

We list the transforms and inverse transforms for the above 8 types. The formulations below have been checked using Python.

1. staggered NN





1. staggered DD





1. staggered ND





1. staggered DN





1. Non-staggered NN





1. Non-staggered DD





1. Non-staggered ND





1. Non-staggered DN





**Appendix D**

We show that on rectangular meshes, FVM and FDM are equivalent. The momentum equation is





Volume integral,





Gaussian theorem,





Here, we assume the cell spacings are non-uniform in the direction. Due to second-order spatial accuracy, the volume average of is equal to the cell-center value. The FDM discretization multiplied by volume





This form can be interpreted as FVM if

1. and is interpreted as volume average (or volume-center value). Since the grid spacings are non-uniform in the direction, the location of is different from the control volume center. Hence, it is better to interpret it as control volume average.

**References**