Introduction to Numerical Methods

Kenn K. Q. Zhang

Fluid mechanics permeates everywhere, in aeronautics, in ship building and offshore structures, in nuclear reactor cooling, in mechanical lubrication, in combustion chamber, in polymer forming, in solidification and material science in general, in aerosol and electro-hydrodynamics, in plasmas physics, in human tissues and blood vessels, and in fluidic micro-channels, just to name a few. Besides the descriptive approach, the means to study fluid mechanics are theoretical, experimental, and computational. The multi-variable, multi-dimension, complex geometry, viscosity, and nonlinearity associated with fluid equations preclude theoretical approach to solve any problem but under simplest idealized circumstances. The theory is useful primarily during the equation system formation, which both the experimental and computational means depend on, and useful in some approximate analytical methods [15] , which occasionally can manage to capture some main features of the flows with omission of details. To solve practical problems, one has to count on experimental and computational means. While experimental approach prevails in fields such as biology and physics, the situation in fluid mechanics is somewhat different, in that fluid motion can be reliably quantified by a set of equations. The Computational Fluid Dynamics (CFD) edges out experiments in several respects.

First of all, CFD predicts flows, and this may be extremely hard for experiments. For instance, weather is forecasted based on software calculations which use measured data as inputs. Experiments would be virtually always behind schedule if being used in this business. Experiments do predict, but are well versed only for something repeatable and do very poorly for real-time situations. Unfortunately for many flows, including that in weather forecasting, the repeatability is virtually always not the case but the simultaneity is virtually always expected from the predicting method. Secondly, CFD has a much closer connection to theory. CFD shares to great extent with theoretical approach during equation system formation, and it separates from theory during system solving stage. So it is sometimes regarded as an arm stretch of the theory. In contrast, experiments rather proceed in their own ways, with less dependency on theory. Hence, CFD can better reveal the underlying mechanism. Thirdly, experiments cannot be applied to certain circumstances. For instance, the magnetohydrodynamics around the sun can be simulated but can not be experimented, and the flow-disturbing support for the aircraft prototype in wind tunnel must be present in experiments but can be removed in CFD simulations. Finally, CFD is much less expensive. The development of a CFD software is expensive and time consuming, but once developed it can be re-used in multiple circumstances and on multiple computers. Also, when solving a new problem an experimental setup typically takes much longer time than CFD. Moreover, CFD is reversible, in that the computer code can go back to certain earlier stage by recovering data. On the contrary, experiments or physical processes often cannot be reversed so that a start from the beginning might be necessary. All these indicate that CFD is much less expensive and in many situations, much more efficient. Therefore, in recent years the demand for CFD has been displaying a monotonic growth and CFD has been recognized as an essential tool in many industrial sectors. Before the motivation of the report is divulged, let us take a look at several aspects of CFD. We begin with the superset of fixed complex geometry.

Symbolically, a differential equation system can be written as

$$L(u) = 0, \tag{1}$$

where L represents any operator and u represents the dependent variable in exact sense. If the exact u (defined at any point in the domain) is replaced by an approximate u_i (defined at selected points), equation (1) is no longer satisfied. Hence, the original system is relaxed to the weak form

$$\int_{\Omega} wL(u_i)d\Omega = 0, \tag{2}$$

where w represents a weight function. Dependent on how the weight function is selected and how the exact u is replaced by u_i, various numerical methods can be generated.

In Eq. (2), if the exact u is replaced by u_i at a set of finite number of points in the space (this is actually equivalent to expressing the exact solution in some specific type of polynomial), and the weight function is selected as the shift function δ_{ij}, then the integral Eq. (2) reduces to

$$L(u_j) = 0$$

This is the Finite Difference Method (FDM). Implicit-in-space FDM is called compact finite difference method [28, Zhang *et al.* 2006]. Straightforward in regular geometry, FDM also features easy implementation for high-order schemes and narrow bandwidth of matrices. FDM can be implemented on structured grid for problems with complex geometry. This is accomplished through a global mapping, which transforms a complex geometry into a regular one, and through boundary fitted coordinates [24, 25]. The other approach to handle complex geometry is the Immersed Boundary Method (IBM) [4, 21]. In Eq. (2), the exact u can be replaced by $u_i\psi_i$, where ψ_i is the Lagrangian interpolation function and u_i is the coefficient. Further, if the weight function is also the Lagrangian polynomial, then it leads to Finite Element Method (FEM). The local geometric mapping, which employs Lagrangian polynomials, was co-born with FEM. In Eq. (2), if the exact u is replaced by u_i as in FDM, but the weight function is selected as unity, then it leads to Finite Volume Method (FVM). FVM is a cell-based conservative method, in contrast to point-based FDM which may not be conservative. After evaluation of cell surface integrals, FVM becomes very close to FDM in the sense of the discrete systems. The most popular FVM grid on regular geometry is clearly the MAC staggered grid [9, 19], which is conservative. Lattice grid was put forth [27, Zhang *et al.* 2006] as another conservative grid. For complex geometry, a variety range of grids/meshes are used [11, 17, for example], however, the MAC staggered grid is hardly seen. The complex geometry may be handled as in Immersed Boundary Method on regular grid [4, Chan & Street], handled via global mapping on structured grid [1, for example], handled locally on unstructured grid as in [11, 17], or handled as in the local geometric mapping approach of FEM. Compared with FDM, discontinuities can be more easily manipulated in FVM though high-order schemes are more difficult to be implemented on FVM.

In Eq. (2), if both the interpolation function and the weight function are spectral polynomials (such as Fourier, Legendre, or Chebyshev), and if Eq. (2) is imposed on the overall domain, then it leads to single-domain Spectral Method (SM) [3]. Spectral methods feature high accuracy, owing to the completeness and orthogonality properties of spectral functions. However, single-domain spectral methods suffer from aliasing, which can be removed but it casts doubts on the desired efficiency of the methods, and from inconvenience for complex geometry, though it is doable with the global mapping as in FDM. In Eq. (2), if both the interpolation function and the weight function are spectral polynomials and imposed on the each element, then it leads to continuous Spectral Element Method (SEM) [7, 13, 6]. The advantage of SEM, which employs the local geometric mapping in FEM, over single-domain spectral method mainly resides in complex geometry handling. Also, very high-order spectral polynomials in single-domain approach is replaced by relatively lower-order (though still high compared with FEM or FVM) polynomials on multiple elements, which is the h/p approach. The performance evaluation of h/p spectral versus single-domain spectral has drawn attention [13, and many others], however, single-domain spectral continues to be the dominant method in turbulence simulations. Thus, a solid evaluation is still in need. A continuous Spectral Element Method with inter-element flux control is named Discontinuous Spectral Element Method (DSEM) [14, 22, 12, 5, 8] . DSEM prevails over SEM in conservation, discontinuity, and parallelization handling.

In Eq. (2), if the Lagrangian polynomial is retained as the interpolation function, but the weight function is selected as the fundamental solution to the operator L, the weak form originally imposed on the interior of the domain is then transformed into integrals on the overall boundary. This leads to Boundary Element Method (BEM) [2, 23]. Different from all previous methods, the primary working place of BEM is the boundary of the domain, not the domain itself. Thus, BEM is regarded as an indirect domain solver, while above mentioned methods belong to the category of direct solvers. BEM is well known for its limitation to linear operators. To handle nonlinearity, BEM has to be combined with a direct domain solver [26, for example]. BEM is also well known for dense influence matrix which hampers the efficiency in 3D calculations, though the dimensionality has been reduced by one. However, it achieves high accuracy for problems where unknowns on boundaries are what exactly to be sought. Owing to reduction of dimensionality, BEM enjoys simplicity in moving boundary problems. In Boundary Element Method, if the interpolation polynomial is replaced by spectral functions, then it leads to Spectral Boundary Element Method (SBEM) [20, 18, 10, 16]. SBEM is a least known numerical method.

For parallel simulation of free-surface flows and for demonstration of important or moderate innovations to be presented in this report, an underlying domain solver must be selected. BEM and SBEM are ruled out immediately because they alone cannot solve incompressible flows, which is nonlinear. Spectral-based methods are ruled out next. Certainly, they are highly accurate. However, these methods alone are still the subject of active research and cost a great deal of time to study, evaluate, innovate, and implement, so that it is impractical to convey the new messages on parallel simulation of free-surface flows within the limited time frame. Also, spectral-based methods require a lot more mathematical skills to understand and are rather repulsive to practical CFD activists, so that innovations bundled with such domain solvers will be hard to disseminate. Furthermore, the treatments related to moving meshes and the free-surface tracking typically are not in high order accuracy, so that the power of spectral-based methods will be hard to show off. FDM is ruled out easily simply because of its deficiency in geometric versatility. Then, it narrows down to FVM and FEM only, and either could be an excellent pick for the current purpose. The weighted integral approach of FEM represents a more general methodology and better posed for future extension to SBEM and DSEM. And, FVM is more popular in CFD, but overall speaking FEM is more renowned in scientific computing of continuum. Thus novelties conveyed on the FEM vehicle can be better disseminated. Finally, the local conservation makes parallelization relatively easy with FVM, and parallelization in FEM remains an arduous task. Hence, the new parallelization method proposed in this report not only meets the need for FEM, but also promises a great success with other domain solvers where parallelization is relatively easy. Due to all these reasons, FVM is ruled out and that leaves FEM as the pick. However, it must be emphasized that the novelties introduced in this report certainly are not expected to be restricted to FEM. They are mutually independent to each other.

References

[1] P. Ananthakrishnan. Radiation hydrodynamics of floating vertical cylinder in viscous fluid. *Journal of Engineering Mechanics*, 125:836–847, 1999.

[2] P. K. Banerjee. *The Boundary Element Methods in Engineering.* McGraw-Hill College, 1994.

[3] C. Canuto, M. Y. Hussaini, A. Quarteroni, and T. A. Zang. *Spectral Methods in Fluid Dynamics.* Springer-Verlag, 1987.

[4] R. K. C. Chan and R. L. Street. A computer study of finite-amplitude water waves. *Journal of Computational Physics*, 6:68–94, 1970.

[5] B. Cockburn, G. E. M. Karniadakis, and C. W. Shu, editors. *Discontinuous Galerkin Methods.* Springer, 1999.

[6] M. O. Deville, P. F. Fischer, and E. H. Mund. *High-Order Methods for Incompressible Fluid Flow.* Cambridge University Press, 2002.

[7] P. F. Fischer. *Spectral Element Solution of Navier-Stokes Equations on High Performance Distributed-Memory Parallel Processors.* PhD thesis, Massachusetts Institute of Technology, 1989.

[8] J. E. Flaherty, L. Krivodonova, J. F. Remacle, and M. S. Shephard. Aspects of Discontinuous Galerkin methods for hyperbolic conservation laws. *Finite Elements in Analysis and Design*, 38:889–908, 2002.

[9] F. H. Harlow and J. F. Welch. Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface. *Physics of Fluids*, 8:2182–2189, 1965.

[10] L. R. Hill and T. N. Farris. Fast fourier transform of spectral boundary elements for transient heat conduction. *Int. J. Num. Meth. Heat Fluid Flow*, 5:813–827, 1995.

[11] C. W. Hirt, A. A. Amsden, and J. L. Cook. An arbitrary Lagrangian-Eulerian computing method for all flow speeds. *Journal of Computational Physics*, 14:227–253, 1974.

[12] G. B. Jacobs. *Numerical simulation of two-phase turbulent compressible flows with a multidomain spectral method.* PhD thesis, University of Illinois at Chicago, 2003.

[13] G. E. M. Karniadakis and S. J. Sherwin. *Spectral/hp Element Methods for CFD.* Oxford, 1999.

[14] D. A. Kopriva and J. H. Kolias. A conservative staggered-grid Chebyshev multidomain method for compressible flows. *Journal of Computational Physics*, 125:244–261, 1996.

[15] E. Lauga. *Slip, Swim, Mix, Pack: Fluid Mechanics at the Micron Scale.* PhD thesis, Harvard University, 2005.

[16] G. P. Muldowney and J. J. L. Higdon. A spectral boundary element approach to three-dimensional Stokes flow. *Journal of Fluid Mechanics*, 298:167–192, 1995.

[17] B. Niceno and E. Nobile. Numerical analysis of fluid flow and heat transfer in periodic wavy channels. *International Journal of Heat and Fluid Flow*, 22:156–167, 2001.

[18] J. M. Occhialini, G. P. Muldowney, and J. J. L. Higdon. Boundary integral/spectral element approaches to the Navier-Stokes equations. *International Journal for Numerical Methods in Fluids*, 15:1361–1381, 1992.

[19] S. V. Patankar. *Numerical Heat Transfer and Fluid Flow.* Hemisphere, Washington, DC, 1980.

[20] A. P. Peirce, S. Spottiswoode, and J. A. L. Napier. The spectral boundary element method: a new window on boundary elements in rock mechanics. *Int. J. Rock Mech. Min. Sci. & Geomech. Abstr.*, 29(4):379–400, 1992.

[21] C. S. Peskin. Numerical analysis of blood flow in the heart. *Journal of Computational Physics*, 25:220, 1977.

[22] D. Stanescu. *A multidomain spectral method for computational aeroacoustics.* PhD thesis, Concordia University, 1999.

[23] C. Wang and B. C. Khoo. An indirect boundary element method for three-dimensional explosion bubbles. *Journal of Computational Physics*, 194:451–480, 2004.

[24] R. W. Yeung and P. Ananthakrishnan. Oscillation of a floating body in a viscous fluid. *Journal of Engineering Mathematics*, 26:211–230, 1992.

[25] R. W. Yeung and P. Ananthakrishnan. Viscosity and surface-tension effects on wave generation by a translating body. *Journal of Engineering Mathematics*, 32:257–280, 1997.

[26] D. L. Young, J. T. Chang, and T. I. Eldho. Solution of three-dimensional unsteady external flow using a coupled arbitrary lagrangian fem-bem model. *Engineering Analysis with Boundary Elements*, 28:711–723, 2004.

[27] K. K. Q. Zhang, B. Rovagnati, Z. Gao, W. J. Minkowycz, and F. Mashayek. An introduction to lattice grid. *Numerical Heat Transfer Part B-Fundamentals*, 51:415–431, 2007.

[28] K. K. Q. Zhang, B. Shotorban, W. J. Minkowycz, and F. Mashayek. A compact finite difference method on staggered grid for Navier-Stokes flows. *International Journal for Numerical Methods in Fluids*, 52:867–881, 2006.