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6. AUTHOR(S)
Thomas Y. Hou, Principal Investigator

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Applied Mathematics, 217-50
California Institute of Technology
Pasadena, CA 91125

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Final Report on ONR Grant N00014-94-1-0310
Thomas Y. Hou (PI)
Applied Mathematics
Caltech, Pasadena

My research works under the support of the ONR grant can be classified into two major areas. One is to develop an adaptive base finite element method for computing multiple scale solutions arising from material science and turbulent transport [7,8]. The other is to develop stable and efficient numerical methods to compute free surface flows in two and three space dimensions [1].

1. An adaptive base finite element method for multiple scale solutions

Many problems of fundamental and practical importance have multiscale solutions. Composite materials and turbulent transport in high Reynolds number flows are examples of this type. Due to the limited computational resources, it is usually impossible to completely resolve all small scale components in the solution. On the other hand, From an engineering perspective, it is often sufficient to predict the macroscopic properties of these systems, such as effective conductivity, elastic moduli, permeability, and eddy diffusivity, and to capture the *averaged* effect of small scales on the large scales. The challenging question is: Can we capture the large scale property correctly without completely resolving all the small scale components?

In this work [7,8], we develop a new method of computing multi-scale and multicomponent problems in composite materials and turbulent transport problems. The new method is based on a general theory of G-convergence of differential operators with multiple scale structure. In this method, the base functions are constructed in such a way that they contain the local microscopic properties of the differential operators. Typically the size of the element is larger than a certain cut-off scale of the oscillatory coefficient, information at smaller scales are built into the base functions. The small scale information in the base functions are brought into the large scale (i.e., grid scale or larger) solution through the coupling of the global stiffness matrix. Thus, the large scale solution is correctly captured. In this sense, we say that the base functions are *adaptive* to the differential operator.

In general, the adaptive base functions need to be constructed numerically except for certain special cases, such as piecewise constant coefficients or space-separable problems. Since the construction is a local operation within the elements, it can be done in perfectly parallel. In effect, we break a large scale computation into many smaller and independent pieces; this is in contrast to traditional domain decomposition methods, in which the pieces are coupled together. Thus, the method is automatically adapted to parallel computers. Moreover, once the small scales information within an element (a base function) is gathered into the global stiffness matrix, the computer memory used for those base functions can be reused for constructing bases of the next element. The ability to gather the fine scale information in such a sequential manner leads to drastic saving of computer memory. This makes it possible for the method to tackle much larger practical problems than the direct numerical methods. Clearly, when the small scale features are localized in a region, we need only to construct the adaptive bases in that region. Therefore, the adaptive-base method can

be used as an alternative to the h-p finite element method or the adaptive mesh refinement methods when the averaged effect of the small scales are of the main concern. Another feature of our approach is that it can handle general multi-scale problems without the requirement of scale separation, a property which is very important for practical applications. Our numerical experiments convincingly demonstrate this effect.

Convergence analysis of our adaptive finite element method is a difficult task. Analysis for conventional finite element methods can not be used to analyze our adaptive method. A more refined analysis which takes into account the microscale structures of the solution is required to reveal the convergence property of our method. In the case of periodic multi-scale oscillatory coefficients, we have been able to demonstrate the convergence of our method. Our analysis shows that the adaptive method converges independent of the small scale feature of the solution [8]. In a subsequent paper, we have carried out a number of careful performance studies using massively parallel super computers. Comparison with other existing numerical methods is also made. Our study shows that our method is very competitive with other numerical methods. Our method can compute multiscale solutions of small scales that are one or two orders magnitude smaller than scales that can be computed by conventional methods. And the overhead in computing the oscillatory bases function only double the amount of works required for a conventional finite element method. To demonstrate the adaptivity and the robustness of our method, we have computed random oscillatory coefficient with fractal dimensions for practical problems in composite materials and porous media flows. Convergence is observed in all our numerical experiments [7]. In the future, we plan to use our method to study the effective conductivity of certain composite materials with large aspect ratio and many unseparable small scale. We will also study wave propagation in random media and the effective diffusivity and possible anomalous diffusion in turbulent transport problems.

2. Efficient and stable numerical methods for free surface flows

Many physically interesting problems involve propagation of free surfaces. Thin film growth for manufacturing materials for electronic devices, solidification problem for crystal growth, Hele-Shaw cells for pattern formation are some of the significant examples. These problems present a great challenge to physicists and applied mathematicians because the underlying problem is very singular. The physical solution is sensitive to small perturbations. Straight-forward discretizations may lead to numerical instabilities. Moreover, in many situations, the numerical modeling is especially difficult due to the presence of topological changes or formation of singularities in the surface. For example, in crystal growth and thin film growth, an initial smooth front can develop cusps and crack-like singularities, and isolated islands of film material can merge. Another difficulty is due to the presence of surface tension in the free surface. It introduces a very stiff term through the local mean curvature. In the case of thin film growth, the situation is even worse. The normal velocity of the free surface is proportional to the second derivative of the local curvature. This would pose an extremely severe stability constraint for time integration if an explicit scheme is used.

In collaboration with Lowengrub and Shelley [2], we introduce a novel idea to remove the stiffness of surface tension by reformulating the problem in the tangent angle and the arclength metric variables. Using this reformulation, we can decompose the small scale

features and integrate the most singular part of the equations implicitly. Our reformulation enables us to invert the implicit solution explicitly by FFT, this greatly improves the speed of the time integration. For computations of the vortex sheet roll-up in an Euler flow with surface tension using a modest number of points (128), the time-step can be chosen 250 times larger than for an analogous explicit method. Many problems which were previously unobtainable now become tractable using our techniques and new phenomena were discovered. Using our reformulated method, a new type of topological singularity was found numerically for fluid interfaces with surface tension, which is different from the curvature singularity due to the Kelvin-Helmholtz instability. A careful numerical study has been recently carried by us to study the scaling property of this pinching singularity using a high order adaptive version of our reformulated boundary integral method [3]. A number of interesting physical phenomena are revealed. Numerical study of the two-density unstably stratified flow with surface tension has also been carried in a joint work with my student, Hector Ceniceros [4]. Our study shows that a similar pinching singularity is also observed in the roll-up of the free surface. The type of singularity is qualitatively similar to the ones we observed for the vortex sheet with surface tension. Convergence of the reformulated boundary integral method has been obtained using delicate energy estimates.

Another significant result we obtained is to develop and analyze a stable, high order 3-D boundary integral method for computing water waves [9,10]. The stability analysis of a 3-D boundary integral method is much more difficult and subtle than its 2-D counterpart. For a 3-D problem, the singular kernel has an un-removable branch point singularity. Moreover, it is much more difficult to obtain the spectral property of the singular integral operators with variable coefficients. In our analysis, we develop a framework under which spectral properties of various singular operators can be analyzed precisely. We found that the 3-D boundary integral method is generically unstable. Using a delicate stability analysis, we show how to remove this numerical instability and construct a stable method for computing 3-D water waves.

In an effort to compute through topological singularity beyond the pinching of the interface, we derive a level set formulation for incompressible, immiscible Navier-Stokes equations separated by a free surface [5]. This is done in collaboration with Chang, Merriman and Osher. The flow we consider has discontinuous density and viscosity. The effect of surface tension is also included. Based on this formulation, a second order projection method can be used to approximate the evolution equations. This approach can be considered as a method of front capturing type since no explicit information about the free surfaces is required in the solution procedure. The free surface is recovered at the end of the computation by locating the zero level set of a smooth function. This numerical method is efficient and is capable of simulating incompressible flow where change of topology in the fluid interface occurs, such as merging and reconnection. An area-preserving re-initialization procedure is introduced to prevent loss of mass due to numerical diffusion. This property is essential for many practical applications. Recently, we (with Osher) have obtained an improved level set formulation for vortex sheets with surface tension [6]. In this formulation, the singular delta function is factored out from the evolution equation. This gives a more robust formulation for both theoretical and computational study. We intend to perform a careful numerical study and compare with the result obtained by using our reformulated boundary integral method. The advantage of using the level set method is that we can compute beyond the

pinching singularity without any difficulty.

Publications and Work in Preparation

1. T. Y. Hou, *Numerical Solutions to Free Boundary Problems,* Acta Numerica, 1995, pp. 335-415.

2. T. Y. Hou, J. Lowengrub and M. Shelley, *Removing the Stiffness from Interfacial Flows with Surface Tension,* J Comput Phys, Vol. 114, 1994, pp. 312-338.

3. T. Y. Hou, J. Lowengrub and M. Shelley, *The Long-Time Motion of Vortex Sheets with Surface Tension,* accepted by Physics of Fluids, A.

4. H. D. Ceniceros and T. Y. Hou, *Convergence of a Non-Stiff Boundary Integral Method for Interfacial Flow with Surface Tension,* accepted by Mathematics of Computation.

5. Y. C. Chang, T. Y. Hou, B. Merriman, and S. Osher, *Eulerian Capturing Methods Based on a Level Set Formulation for Incompressible Fluid Interfaces,* J. Comp. Phys., Vol. 124, pp. 449-464, 1996.

6. T. Y. Hou, and S. Osher, *An Improved Level Set Formulation for Vortex Sheets with Surface Tension,* in preparation.

7. T. Y. Hou and X. H. Wu, *An Adaptive-Base Method for Elliptic Multiple Scale Problems in Composite Materials and Porous Media,* preprint, submitted to J. Comp. Phys.

8. T. Y. Hou, X. H. Wu, and Z. Cai, *Convergence of An Adaptive-Base Method for Elliptic Problems with Rapidly Oscillating Coefficients,* preprint, submitted to Math. of Comp.

9. T. Y. Hou, Z. H. Teng, and P.W. Zhang, *Well-Posedness for Linearized Motion of 3-D Water Waves far from Equilibrium* accepted by Comm. in P.D.E.

10. T. Y. Hou and P.W. Zhang, *Stability of Boundary Integral Methods for 3-D Water Waves,* in preparation.