RESEARCH STATEMENT

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My research falls into the general area of computational and applied mathematics, including mathematical modeling, applied analysis, numerical analysis and scientific computing. Efficient numerical methods for partial differential equations (PDEs) are central to many disciplines in mathematics, engineering, physics, and biology, etc. Its diverse world of applications spans fluids dynamics, plasma, semiconductors and biomolecules. This is a high leverage field and the achievements in efficient numerical methods can have far-reaching impacts on many other disciplines. As shown by my publications list, I have already accumulated some experience and skills in developing numerical methods as well as their efficiency analysis.

1. Past and current research summary

For the Poisson-Boltzmann (PB) equation, which is a nonlinear elliptic equation, I proposed a high order iterative discontinuous Galerkin (DG) method, which was recognized as the first DG method to solve the PB equation. Another problem involving the elliptic equation is the Poisson–Nernst–Planck (PNP) system, one main challenge for developing numerical schemes for the PNP system is to ensure density positivity, I proposed a positivity-preserving third order DDG method, which is the first positivity-preserving third order numerical method for the PNP system. The elliptic equation with line Dirac sources generally admits a singular solution, hence, the convergence rate of the finite element method (FEM) is sub-optimal. I proposed a finite element algorithm, which is of optimal convergence rate. Please see my papers [15, 16, 1, 12].

For time-dependent fourth order problems, I proposed a penalty free DG method, and I further applied this DG method to solve a class of fourth order gradient flows, these problems are challenging because of the interplay between the higher-order diffusion and nonlinearity on one hand, and the presence of a Lyapunov functional on the other. I have developed several methods to solve the fourth gradient flows, such as the IEQ-DG method, the SAV-DG method, and the LEQRK-DG-PC method, while the last one is the first unconditionally energy stable method of arbitrarily high order within the DG framework. All proposed schemes are unconditionally energy stable, linear and easy to implement. Please see my papers [7, 8, 9, 10, 11].

A fast solver generally is the easiest way to solve the high order PDEs. However, its solution is not always reliable due to possible singular issues. For biharmonic equation with Navier boundary conditions in a polygonal domain containing a reentrant corner, the usual mixed finite element formulation produces numerical solutions that converge to a wrong solution. I proposed and analyzed an optimal C^0 finite element algorithm for solving this biharmonic problem, which involves solving an additional intermediate Poisson problem that confines the solution in the correct space. Please see my papers [2, 3].

These research achievements have already created large impacts in my research area, and my articles have been quoted by experts.

Date: Mar. 31, 2021.

2. Research plan

2.1. **Background.** Many phenomena in engineering, physics, and biology can be described by high order PDEs, nonlinear PDEs, or their interplay. For example, the Cahn-Hilliard equation, phase field crystal equation, and the Lifshitz-Petrich equation, these equations are fourth, sixth, and eighth order PDEs, respectively. They have important applications in phase separation, quasi-crystal, etc. Generally, these kinds of equations cannot be solved analytically. Therefore, computer simulations play an essentials role in understanding of the non-equilibrium processing and how it leads to pattern formation.

In order to design a numerical method, a typical way is to rewrite the high order equation into a system of lower order equations. Thus, faster solvers or efficent numerical algorithms could be designed to obtain the numerical solutions. This is the strategy for many numerical methods, such as the mixed element method, mixed interior penalty DG method. Although it has been demonstrated to be successful for many cases, the solutions of the system are not always equivalent to the solution of the original equation, which is known as paradoxes, such as Babuška paradox, Sapongyan paradox, etc. The numerical schemes may not be easy to design due to the existence of a nonlinear term, an unstructured domain, a singular source term, or some special properties of the solution. Whether we can modified the system such that the solutions are equivalent? Whether we can design an efficient or a simple algorithm for the system? Whether the numerical solution still preserve the properties of the original equation if any? We propose to answer these questions by applying some new methods.

2.2. **Proposed work.** Our research concentrates on efficient numerical methods for high order PDEs by rewriting it into a system of lower order equations. We proposed a new approach to deal with the Sapongyan paradox by removing the solution of an additional equation to confine the solution of the system into the same space as the original equation, so that their solutions are equivalent. The approach is shown to be efficient and useful for many cases, such as biharmonic equation with Navier boundary conditions in a polygonal domain. It could be also applied to biharmonic equation with Dirichlet boundary conditions, and sixth order elliptic equation with simply supported boundary conditions. We could also analyze the efficiency and derive the error estimates of the proposed numerical method. Moreover, we can further explore more complicated cases, and extend the approach to other paradoxes.

For time-dependent fourth order PDEs, we proposed a penalty free DG method, and IEQ-DG/SAV-DG method when these equations interplay with nonlinear terms. These methods could be applied more general cases. For example, the penalty free DG method could be extend to eighth order PDEs, and further apply the corresponding IEQ-DG/SAV-DG method to nonlinear cases, such as the Lifshitz-Petrich equation, which has an important application in quasi-crystal. Some error analysis could be carried out for the penalty free DG method when it is applied to equations with different boundary conditions. We can further propose IEQ-FEM and IEQ-enriched Galerkin (EG) method for gradient flows, and also explore the maximum-preserving property and the superconvergence of the EG method, which is a new method inheriting some merits of the DG and FEM method.

I hope to continue pursuing this research work at your institute.

2.3. **Impact of work.** Successful accomplishment of the porposed research will provide efficient and simple numerical schemes for high order equations, especially if there exists a nonlinear term, an unstructured domain, a singular source term, or some special properties of the solution. This research will also provide a constructive method in implementing faster solvers, and will be beneficial to many disciplines in mathematics, engineering, physics, and biology, etc.

3. Statement of Research Interests

3.1. Numerical methods for the second order elliptic PDEs.

3.1.1. *The nonlinear Poisson-Boltzmann equation.* For the nonlinear Poisson-Boltzmann (PB) equation, which has many applications, including semiconductor modeling and charged particles in solutions, we proposed a high order iterative discontinuous Galerkin (IDG) method [15], which resolves two main challenges, one is nonlinearity of the model, and the other is smallness of the parameter $\lambda \ll 1$ in the model. We rigorously derived the error estimates for the IDG method in [16]. The IDG method was recognized as the first DG method to solve the PB equation.

3.1.2. *Elliptic equations with singular sources.* Elliptic equations with line Dirac sources occur in monophasic flows in porous media or drug delivery in the network of blood vessels. Since the source term is not an L^2 function, the solution is merely in $H^{\frac{3}{2}-\epsilon}(\Omega)$ for $\epsilon > 0$, which implies the standard error estimate yields only a sub-optimal convergence rate. In [1], we derived regularity estimates in a class of Kondratiev-type weighted spaces and proposed optimal finite element algorithms. Based on the new regularity results, we further proposed graded mesh refinement algorithms, such that the associated finite element methods (FEMs) of any order recover the optimal convergence rate even when the solution is singular.

3.2. Discontinuous Galerkin method for time-dependent PDEs.

3.2.1. *Penalty free DG method for fourth order PDEs.* In literature, the DG methods for the fourth order PDEs are usually discretized by the interior penalty DG (IPDG) method or local DG (LDG) method which is to rewrite the equation into a first order system. For the latter, one has to compute three additional auxiliary variables. In [7], we proposed a mixed DG method **without interior penalty** (or penalty free DG method). The resulting scheme is the most simple variant to date for the discretization of second order terms, i.e., without any interior penalty. This is in sharp contrast to the IPDG method and the DDG methods introduced in [5, 6] for diffusion, where interface corrections are included to penalize jumps of both the numerical solution or its second order derivatives. For the proposed penalty free DG method, we showed its L^2 stability and presented the optimal L^2 error estimate of order $O(h^{k+1} + (\Delta t)^2)$ for fully discrete DG schemes.

3.2.2. *DG method for the fourth order gradient flows.* The fourth order gradient flows describes important physical processes in nature, and it requires very large time simulations to reach steady states. An explicit time discretization may require a time step extremely small to keep the energy dissipation (see e.g. [14]). We proposed various efficient numerical methods to solve the fourth order gradient flows.

Integration of EQ formulation with DG for solving the fourth order gradient flows began with my work [8], where up to 2nd order (in time) **IEQ-DG schemes** were introduced. A key point for the success in the scheme formulation is that the auxiliary energy variable is updated in pointwise manner, and then it is projected back into the DG space. Later, we further extended the strategy of constructing the IEQ-DG schemes to solve the Cahn-Hilliard equation [10], where the spatial discretization is based on the DDG method [5, 6]. We noted that a direct integration of the DG method with the SAV approach [13] would lead to linear systems involving dense coefficient matrices, hence rather expensive to solve. We introduced a special procedure in [9] as a rescue, so the resulting **SAV-DG schemes** become well positioned.

Additionally, we also constructed unconditionally energy stable DG schemes coupled with arbitrarily high order time discretization in [11]. Firstly, starting from a semi-discrete DG scheme of from, we reformulated an extended linearized ODE system by the energy quadratiztion (EQ) approach. Secondly, we applied an s-stage algebraically stable RK method for temporal discretization. The resulting fully discrete **LEQRK-DG-PC schemes** are shown to be unconditionally energy stable. The existing literature works are based on the time discretization of the PDE system first. In contrast, my starting point is a nonlinear ODE system in the form of a semi-discrete DG scheme, this requires new techniques in both the scheme formulation and the proof of the scheme properties. The proposed method is the **first** unconditionally energy stable method of arbitrarily high order within the DG framework for the gradient flows.

3.3. **Maximum principle preserving numerical methods.**

3.3.1. *Positivity-preserving third order DDG method for the PNP system.* The Poisson–Nernst–Planck (PNP) system has been widely used to describe drift and diffusion phenomena for a variety of devices, including biological ion channels and semiconductor devices. However, the PNP system is nonlinear and strongly coupled, efficient computation of it is highly non-trivial. One main challenge for developing numerical schemes for the PNP system is to ensure density positivity (or non-negativity), since negative ion concentrations would be non-physical. In [12], we proposed a positivity-preserving third order DDG method, which is of third order in space and features a provable positivity-preserving property. Its key feature lies in numerical flux choices for the solution gradient, which involves interface jumps of both the solution, and the second order derivatives. In the literature, the proposed method is the first positivity-preserving third order numerical method for the PNP system.

3.4. **Fast solvers for the high order PDEs.** A fast solver generally is the easiest way to solve the high order PDEs. However, its solution is not always reliable due to possible singular issues.

3.4.1. *A C^0 FEM for the biharmonic problem.* The biharmonic equation with Naiver boundary conditions

$$\Delta^2 u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{and} \quad \Delta u = 0 \quad \text{on } \partial\Omega, \tag{3.1}$$

occur for example in the model for the static loading of a pure hinged thin plate. When the domain possesses reentrant corners, however, the usual mixed finite element formulation produces numerical solutions that may be converging but to a wrong solution [17].

In [2, 3], we proposed and analyzed a C^0 finite element method for solving the biharmonic problem (3.1). In particular, we devised an explicit mixed formulation to transform equation (3.1) into a system of three Poisson equations. This is based on the observation that the aforementioned usual mixed formulation (decomposition into two Poisson equations) in fact defines a weak solution in a larger space than that for equation (3.1). This mismatch in function spaces does not affect the solution in a convex domain; while in a non-convex domain, it allows additional singular functions and therefore results in a solution different from that in equation (3.1). The proposed mixed formulation ensures that the associated solution is identical to the solution of (3.1) in both convex and non-convex domains. This is accomplished by the additional intermediate Poisson problems that confine the solution in the correct space. In addition, we carefully derived the optimal error estimates for the proposed method.

Summary

In a summary, I expect to tap into my last few years working experience as a gradient students and a postdoctoral fellow in establishing a comprehensive research effort geared primarily towards designing efficient numerical methods for high order PDEs, especially if there exists a nonlinear term, an unstructured domain, a singular source term, or some special properties of the solution. Both research directions can begin with a comprehensive effort comprising mathematical techniques, theory and methods. The rough time scale to get command of the theorem and methods in this research is about one year. Within one year, I anticipate that I will be carrying out solution analysis and comparing my theory and method with the results in the literature. On the basis of my research experience researched academic achievements, I am very condiment that I can attach external funding. When appropriate, I will seek to collaborate with researches at Iowa State University, Wayne State University, Xiangtan University, Florida State University, and at other organizations so as to carry out a broad research effort.

References

[1] H. Li, X. Wan, P. Yin and L. Zhao. Regularity and finite element approximation for two-dimensional elliptic equations with line Dirac sources. *Journal of Computational and Applied Mathematics*, 393:113518, 2021.

[2] H. Li, P. Yin, and Z. Zhang. A C^0 finite element method for the biharmonic problem with Navier boundary conditions in a polygonal domain. *SIAM J. Numer. Anal.*, to appear, 2021.

[3] H. Li and P. Yin. Optimal high-order C^0 finite element method for the biharmonic problem with the hinged boundary condition. *SIAM J. Numer. Anal.*, submitted, 2021.

[4] H. Liu, J. Ralston and P. Yin. General Superpositions of Gaussian beams and propagation error. *Math. Comp.,* submitted.

[5] H. Liu and J. Yan. The Direct Discontinuous Galerkin (DDG) method for diffusion problems. *SIAM J. Numer. Anal.*, 47(1):675–698, 2009.

[6] H. Liu and J. Yan. The Direct Discontinuous Galerkin (DDG) method for diffusion with interface corrections. *Commun. Comput. Phys.*, 8(3):541–564, 2010.

[7] H. Liu and P. Yin. A mixed discontinuous Galerkin method without interior penalty for time-dependent fourth order problems. *J. Sci. Comput.,* 77:467–501, 2018.

[8] H. Liu and P. Yin. Unconditionally energy stable DG schemes for the Swift-Hohenberg equation. *J. Sci. Comput.,* 81:789-819, 2019.

[9] H. Liu and P. Yin. Unconditionally energy stable DG schemes for the Cahn-Hilliard equation. *Journal of Computational and Applied Mathematics*, 390:113375, 2021.

[10] H. Liu and P. Yin. On the SAV-DG method for a class of fourth order gradient flows. *arXiv preprint,* arXiv: 2008.11877, 2020.

[11] H. Liu and P. Yin. Energy stable Runge-Kutta discontinuous Galerkin schemes for a class of fourth order gradient flows. *arXiv preprint, arXiv:2101.00152*, 2021.

[12] H. Liu, Z. Wang, P. Yin and H. Yu. Positivity-preserving third order DG schemes for Poisson–Nernst–Planck equations. *arXiv preprint, arXiv:2102.00101*, 2021.

[13] J. Shen, J. Xu and X. Yang. The scalar auxiliary variable (SAV) approach for gradient flows. *J. Comput. Phys.*, 353:407–416, 2018.

[14] H. Xi, J. Viñals and J. D. Gunton. Numerical solution of the Swift-Hohenberg equation in two dimensions. *Physica A: Statistical Mechanics and its Applications,* 177:356–365, 1991.

[15] P. Yin, Y. Huang and H. Liu. An iterative discontinuous Galerkin method for solving the nonlinear Poisson Boltzmann equation. *Commun. Comput. Phys.* 16:491–515, 2014.

[16] P. Yin, Y. Huang and H. Liu. Error estimates for the iterative discontinuous Galerkin method to the nonlinear Poisson-Boltzmann equation. *Commun. Comput. Phys.* 23:168–197, 2018.

[17] S. Zhang and Z. Zhang. Invalidity of decoupling a biharmonic equation to two Poisson equations on non-convex polygons. *Int. J. Numer. Anal. Model.*, 5(1):73–76, 2008.