John Li: Proposed Research

Intellectual Merit: Classical Fluid mechanics studies fluid systems using differential equations. For most realistic fluid systems, the differential equation is nonlinear, and must rely on numerical simulations. Sometimes the spatial grid and time grid requirement to resolve the differential equation is computationally heavy in such a manner that it requires a super computer or is not even possible. Long-term prediction even requires long integration time that cumulates round-off errors. Traditional numerical simulation of fluid systems has many limitations; many alternative approaches to improve the computation cost and accuracy have been proposed for many specific systems.

For the concern of reaction front propagation, many experimental and theoretical works have demonstrated the existence of distinct boundaries for fronts in various dynamical systems. Front propagation in *Reaction-Diffusion* (RD) systems is well described by Fisher-Kolmogorov-Petrovsky-Piskonuv (FKPP) theory. However, such theory for *Advection-Reaction-Diffusion* (ARD) systems is generally lacking. My prior research with Dr. K. Mitchell at UC Merced took a dynamical approach to understand the front propagation in ARD systems and had successfully developed *Burning Invariant Manifold* (BIM) theory [1] to predict the long-term reaction front behavior of two-dimensional ARD fluid systems. Our experimental collaborator group of Prof. T. Solomon at Bucknell University produced experimental images that agree with our simulation [2], which confirms the validity of BIM theory.

In most real cases, this BIM theory on two-dimensional flows has limitations, because many realistic dynamical systems are not time periodic and cannot be modeled as 2D. **The proposed work will develop a generalization of the 2D BIM theory to 3D full model by investigating 1. the bounding property of the invariance manifolds. 2. the bifurcation of fixed points that generates the invariance manifolds.**

The current 2D *Burning Invariant Manifold* (BIM) theory is established on 3D ODE of x, y, θ, where x, y are the 2D real space and θ represents the angle in x-y space which is only one dimensional. In the generalization of 2D BIM theory to 3D, its theoretical framework will be extended to 5D ODE of x, y, z, θ, ϕ, where x, y, z are the 3D real space and θ, ϕ are the spatial angles.

First, we hypothesize reaction fronts will still be bounded by the BIMs (non-trivially), which will be 2D unstable manifolds (*2D BIMs*) in this 3D model. Our approach to prove this hypothesis has three steps. Knowing the fact that not all curves in the 5D phase space are physical fronts, 1. We first need to prove the BIMs in the 5D phase space do represent physical fronts. 2. Under the constant front speed condition, no two fronts can pass each other when they travel in the same direction. 3. For all physical fronts in the limit of converging to a BIM, the front direction will also align with the BIM direction. Proving these three points will prove our hypothesis. We believe our hypothesis is correct because experimental research has widely shown the existence of distinct fronts in general 3D real fluid systems. If our hypothesis is false, we want to investigate if with certain restrictions we can restore this hypothesis.

After we generalize the theoretical framework of the generalized BIM theory, our interest will be on the *2D BIMs* because their 5D phase space projection onto 3D real space will be responsible for bounding the physical fronts. We predict that the *2D BIMs* will be generated from *SSSUU fixed points*, where S U are stable and unstable eigen-directions to be obtained by local linear analysis. Intuitively, we would expect every eigen-direction could be either stable or unstable, giving us a total 6 types of fixed points.

My prior research experience on 2D BIM theory will greatly help me on this proposed work. The study on *bifurcation* of fixed points is about the evolution of fixed points with changing parameters. This is an essential research direction because BIMs are generated from fixed point. In the 5D phase space of 6 types of fixed points, bifurcation will have a rich variety of $C_2^6 = 15$. However, we would not expect all 15 bifurcations to be possible because, as we have already seen in the 2D BIM theory, the bifurcation between certain points are forbidden or non-generic. Such study can be done by analyzing the topological properties on fixed points and explicitly studying the relationship among the eigenvalues of fixed points.

While we can already expect the physical significant of SSSUU fixed points, the role of the other five types of fixed points is still unknown. In fact, their existence is even unknown. In this proposed work, we also want to prove their existence, e.g., by simulation, and find their physical significance. Being proficient in MATLAB allows me to perform numerical simulations to better visually understand the system, and thereby gain intuition to formulate theorems.

In conclusion, because the 3D BIM theory has a much wider variety of fixed points, we do expect to find phenomena that do not exist in the 2D BIM theory through simulation. For example, can the other 5 types of fixed points give rise to bounding properties? Can there exist boundaries that are not a result of 2D manifolds? As verification, once the 3D BIM theory is developed, its 2D limit should exactly agree with our current 2D BIM theory.

Broader Impact: We can broaden the participation of those who enter disciplines in science and technology by lowering the barrier of Math. Although my proposed research does not directly cause much broader impact, the software *Natural-Math* (outlined in personal statement) that I will develop to assist me conduct this theoretical research may cause a wide range impact on education and research. For the software development of *Natural-Math*, I will partner with game programmers for the purpose of user-friendly input—and also to appeal to children in a child-friendly version. Although we now have amazing software like Matlab, Mathematica, and Maple, their user interface is still not ideal due to traditional keyboard-mouse limitation. This explains why many professors refuse to use such software. *Natural-Math* is designed to eliminate boring repetition and give the freedom to play with math to the users with the most efficient interface.

This natural user-interface is also fun for educational purposes. If slicing fruits can be a poplular game on iPad, so can equation manipulation–by moving x, y^2, π, e^z... and canceling terms. It eliminates the boring aspect of math, and helps the development of interest in math at children's early stage of education. For instance, children don't need to worry about accidentally dropping a "minus sign" because every operation must obey math-rules. Up on the maturity of *Natural-Math*, I will make it publicly available because I am deeply devoted to develop it to become as important as Matlab, Mathmatica and Maple, while not simply substituting them but complimenting them on what they do not have. Although iPad and other multi-touch screen products are currently still rare, as the technology progresses, they will be as common as cellphones, allowing everyday use of *Natural-Math*.

References:

[1] Kevin A. Mitchell and John R. Mahoney. Invariant manifolds and the geometry of front propagation in fluid flows. Chaos: *An Interdisciplinary Journal of Nonlinear Science*, 22(3):037104, 2012.

[2] Dylan Bargteil and Tom Solomon. Barriers to front propagation in ordered and disordered vortex flows. Chaos: *An Interdisciplinary Journal of Nonlinear Science*, 22(3):037103, 2012.