

# AMS Standard Cover Sheet

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Granting Institution University of California Irvine Date (optional) 06/2009

Ph.D. Advisor: Prof. Hongkai Zhao

Thesis Title (optional) Numerical Methods for Hamilton-Jacobi Equations

Primary Interest (MSC# only) 65 Secondary Interests (optional) 78, 86

Give a very brief synopsis of your current research interests in the box below (e.g. finite group actions on four-manifolds).

*My current research focus on numerical methods for partial differential equations with applications, especially on (1) multiscale and multiphysics modeling and computation of nano optical responses, nano optics; (2) computational high frequency wave propagation, geometrical optics and beyond; and (3) Hamilton-Jacobi equations with applications, Homogenization.*

<http://math.msu.edu/~luos/>

Most recent position held, if any, post Ph.D.

University or Company Michigan State University

Position Title Visiting Assistant Professor Dates 08/16/2009-08/15/2012

Indicate the position for which you are applying and position posting code, if applicable

NTT

Eligible for positions which requires U.S. citizenship or U.S. permanent residency:  Yes  No

If unsuccessful for this position, would you like to be considered for a temporary position?

Yes  No If yes, please check the appropriate boxes.

Postdoctoral Position  2+ Year Position  1 Year Position

List the names and affiliations of individuals who will provide letters of recommendation if asked.

1. Gang Bao, Michigan State University, bao@math.msu.edu

2. Jean-David Benamou, INRIA, France, jean-david.benamou@inria.fr

3. Di Liu, Michigan State University, richardl@math.msu.edu

4. Jianliang Qian, Michigan State University, qian@math.msu.edu

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November 21, 2011

Search Committee  
Department of Mathematical Sciences  
Fisher 319  
1400 Townsend Drive  
Houghton, MI 49931

Dear Search Committee,

I found on [mathjobs.org](http://mathjobs.org) that your department has an open Tenure-Track position for mathematicians on computational and applied mathematics. I am applying to fill this open position. Currently, I am working on projects of these fields as a Visiting Assistant Professor in the Department of Mathematics at the Michigan State University.

I have strong commitment to research. As you will see in my Research Statement, my current research focuses on (1) multiscale and multiphysics modeling and computation to study optical properties of nanostructures; (2) computational high frequency wave propagation with geometrical optics and beyond; and (3) fast and accurate numerical schemes for the Hamilton-Jacobi equations with applications. Several future projects will be carried out along these directions. I hope my research will contribute to your groups on computational and applied mathematics.

I also love to teach. I am interested in teaching both undergraduate and graduate courses such as all levels of Calculus, Linear Algebra, Numerical analysis, Numerical Partial Differential Equations and other relevant courses on computational and applied mathematics. My experience on teaching calculus and research background will be helpful for the students of different levels.

I have enclosed the AMS cover sheet, my curriculum vitae, including a list of publications and a list of references, research statement and teaching statement.

Please feel free to contact me if you have any questions regarding my application. I am looking forward to hearing from you soon. Thank you very much for the consideration.

Sincerely,

Songting Luo

## Curriculum Vitae

### Songting Luo

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#### EDUCATION

- Ph.D., Mathematics.** University of California, Irvine. 2009  
Supervised by Prof. Hongkai Zhao
- M.S., Mathematics.** University of California, Irvine. 2006
- B.S., Mathematics.** University of Science and Technology of China. 2004

#### ACADEMIC APPOINTMENTS

- 09/2009– Visiting Assistant Professor  
Department of Mathematics and  
Michigan Center for Industrial and Applied Mathematics  
Michigan State University  
Hosted by Profs. Gang Bao, Di Liu and Jianliang Qian
- 09/2004–06/2009 Research Assistant  
Department of Mathematics  
University of California, Irvine

#### RESEARCH

- Multiscale, Multiphysics Modeling and Computation of Nano-Optical Responses; Semiclassical Theory; (Time-Dependent) Density Functional Theory; Nano Optics.
- Computational High Frequency Wave Propagation; Geometrical Optics and Beyond.
- Numerical Methods for Hamilton-Jacobi Equations With Applications; Homogenization.

## TEACHING

- Spring 2010, *MATH132 Calculus*. Michigan State University.  
Fall 2010, *MATH133 Calculus*. Michigan State University.  
Spring 2011, *MATH360 Mathematical Theory of Interest*.  
Michigan State University.  
Fall 2011, *MATH132 Calculus*. Michigan State University.

## PUBLICATIONS & PREPRINTS

### JOURNAL PAPERS & PREPRINTS

1. S. Fomel, S. Luo and H. Zhao, *Fast sweeping method for the factored eikonal equation*, Journal of Computational Physics, Volume 228, Issue 17 (2009) 6440-6455.
2. J. D. Benamou, S. Luo and H. Zhao, *A compact upwind second order scheme for the Eikonal equation*, Journal of Computational Mathematics, Volume 28, No.4, 2010, 489-516.
3. S. Luo, L. J. Guibas and H. Zhao, *Euclidean Skeletons Using Closest Points*, Inverse Problem and Imaging, Volume 5 Issue 1, 95-113 (2011).
4. S. Luo, Y. Yu and H. Zhao, *A new approximation for effective Hamiltonians for homogenizations of a class of Hamilton-Jacobi equations*, Multiscale Modeling & Simulation, Volume 9 Issue 2, 711-734 (2011).
5. S. Luo, S. Leung and J. Qian, *An Adjoint State Method for Numerical Approximation of Continuous Traffic Congestion Equilibria*, Communications in Computational Physics 10, 1113-1131. (2011).
6. S. Luo and J. Qian, *Factored singularities and high-order Lax-Friedrichs sweeping schemes for point-source traveltimes and amplitudes*, Journal of Computational Physics. 230 (2011) 4742-4755.
7. S. Luo and J. Qian, *Fast sweeping method for anisotropic eikonal equations: additive and multiplicative factors*, Journal of Scientific Computing, accepted.
8. S. Luo, J. Qian and H. Zhao, *Higher-order schemes for 3-D first arrival*

*traveltimes and amplitudes*, Geophysics, accepted.

9. G. Bao, D. Liu and S. Luo, *MultiPhysical Modeling and Multiscale Computation of Nano Optical Responses*, Submitted.

10. S. Luo and H. Zhao, *Contraction Property of Fast Sweeping Method*, Submitted.

11. S. Luo and J. Qian *Fast Huygens sweeping method for the Helmholtz equation*, Preprints.

12. G. Bao, D. Liu and S. Luo, *A Multiscale Scheme for the Study of Scanning Near-Field Optical Microscopy*, Preprints.

#### **IN PREPARATION**

13. S. Luo, Y. Yu and H. Zhao, *Fast sweeping schemes for effective Hamilton-Jacobi equations*, in Preparation.

14. S. Luo and J. Qian, *An adjoint state method for inverse attenuation X-ray transform*, in Preparation.

15. S. Luo and J. Qian, *A geometrical optics approach to Maxwell equations within high frequency regime with factored singularities*, in Preparation.

16. G. Bao, D. Liu, S. Luo and C. Yang, *Numerical study of self-assembly of quantum dots by Maxwell-TDDFT approach with parallel implementation*, in Preparation.

#### **THESIS**

S. Luo, *Numerical Methods for Hamilton-Jacobi Equations*, June 2009, Ph.D Thesis, University of California, Irvine.

S. Luo, *The Symmetry Group of the Kadomtsev-Petviashvili Equation with Self-Consistent Sources and the Deformation of One Soliton Solution Under the Symmetry Group*, June 2004, B.S. Thesis, Supervised by Prof. Xiaoda Ji, University of Science and Technology of China, China.

#### **CONFERENCES & PRESENTATIONS**

- Symposium at the University of Michigan, Nonlinear Optics At 50. (October 2011)
- Michigan Center for Industrial and Applied Mathematics Workshop on Computational Wave Propagation, invited talk “Factored Singularities for Traveltime and Amplitude”. (April 2011)
- Michigan Center for Industrial and Applied Mathematics Workshop on Multiphysics Modeling and Computation of Nano-Optical Response, invited talk “Multiphysics Modeling and Computation of Nano-Optical Response”. (March 2011)
- Banff Workshop on Advancing Numerical Methods for Viscosity Solutions and Applications, International Research Station, Canada. (February 2011)
- SIAM Annual Meeting, invited talk “A new approximation for Effective Hamiltonians”. (July 2010)
- IMA Summer School on Computational Wave Propagation, Michigan State University. (June 2010)
- Michigan Center for Industrial and Applied Mathematics Workshop on Inverse Problems: Theory, Computation and Application. (April 2010)
- Banff Workshop on Recent Developments in Numerical Methods for Non-linear Hyperbolic Partial Differential Equations and their Applications, International Research Station, Canada. (September 2008)
- SIAM Annual Meeting, invited talk “Compact Upwind Second Order Scheme for Eikonal Equation”. (July 2008)

## REFERENCES

- |                         |   |
|-------------------------|---|
| Dr. Gang Bao,           | Michigan State University, <a href="mailto:bao@math.msu.edu">bao@math.msu.edu</a>           |
| Dr. Jean-David Benamou, | INRIA, France, <a href="mailto:Jean-David.Benamou@inria.fr">Jean-David.Benamou@inria.fr</a> |
| Dr. Di Liu,             | Michigan State University, <a href="mailto:richardl@math.msu.edu">richardl@math.msu.edu</a> |
| Dr. Jianliang Qian,     | Michigan State University, <a href="mailto:qian@math.msu.edu">qian@math.msu.edu</a>         |
| Dr. Chao Yang,          | Lawrence Berkeley National Laboratory, <a href="mailto:cyang@lbl.gov">cyang@lbl.gov</a>     |
| Dr. Hongkai Zhao,       | University of California, Irvine, <a href="mailto:zhao@math.uci.edu">zhao@math.uci.edu</a>  |

# Research Statement

Songting Luo \*  
 Department of Mathematics  
 Michigan State University

## 1 Overview

My current research focuses on numerical methods for partial differential equations with applications, especially,

- (1) multiscale and multiphysics modeling and computation of nano optical responses with applications to nano optics;
- (2) computational high frequency wave propagation, geometrical optics and beyond;
- (3) numerical methods for Hamilton-Jacobi equation and its applications to geophysics.

In the following, I will briefly describe each of these projects along with future goals.

## 2 Multiscale and Multiphysics Modeling and Computation of Nano Optical Responses

The study of radiation-matter interaction of nanostructures has attracted numerous interests in the development of modern physics with many practical applications, e.g. in nanoscience and nanotechnology. The quantum electrodynamics (QED) [11] can give a complete description of the interaction but its intensive computational expense limits its potential applications. The semiclassical theories [10, 22, 43] can describe many physical processes as well as QED does and the high computational cost is reduced through the classical treatment of the electromagnetic (EM) field and the first principle approach for the charged particles. However, a many-body Schrödinger equation is still involved, which is in general prohibitive to solve either analytically or numerically.

### 2.1 Our approach: work in [4, 3]

Our work [4, 3] is designed to propose a multiscale scheme to numerically study the nano optical response by combining the semiclassical theory [10] and the density functional theory (DFT) and its time-dependent analogue, the time-dependent (current) density functional theory (TD(C)DFT) [41, 17]. We utilize Cho's semiclassical theory, where the evolution of the EM field is determined classically by the microscopic Maxwell equations and the motion of the matter system ( $N$  electrons) is governed by the Schrödinger Equations, through which the EM field, current density and charge density are coupled and must be determined self-consistently. The high cost of solving the many-body Schrödinger Equations is resolved with the DFT and TD(C)DFT which treat the single particle density and/or current density as basic variables and avoid calculating the many-body wavefunctions. Moreover the single particle density and/or current density can be obtained through the Kohn-Sham (KS) system which is a system of single particle Schrödinger Equations, hence it can be solved with much lower cost [23].

We incorporate the linear response theory within TD(C)DFT [44, 9] into Cho's linear response formulation [10] to study the optical response of nanoscale systems. A linear system for self-consistently determining the

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induced EM field (by Maxwell equations), induced current density and induced density (by KS system) is obtained, and can be put in a compact form,

$$(\mathcal{S} - \omega^2 \mathbf{I})\mathcal{P} = \mathcal{F}_0, \quad (1)$$

by introducing the P-matrix  $\mathcal{P}$ , where  $\mathcal{S}(\omega)$  contains the exchange-correlation effects, the Hartree potential and the radiative correction (see [4, 3] for derivations), and  $\mathcal{F}_0$  relates to the incident field. The eigenmodes exist for particular frequencies such that the matrix in (1) is degenerate. The resonant structure of optical spectra corresponds in general to eigenfrequencies of such modes of the radiation-matter system. Therefore we study the optical property of the system by

- Compute eigenfrequencies by solving the zero eigenvalue problem:  $\mathcal{S} - \omega^2 \mathbf{I}$  has a zero eigenvalue. We design an iterative Jacobi-Davidson scheme (e.g. [1]) to compute the eigenmodes.
- Determine the EM field, density and current density for given frequency by solving (1). A BiCGSTAB algorithm [45] is used.

The coupled linear system has a multiscale nature, i.e. the macro scale for the EM field and the micro scale for the electron and current densities. We design a multiscale method which consists of a **macro solver** for the Maxwell equation (Finite Element Method [21] or Finite Difference Frequency Domain Method [19]) and a **micro solver** based on DFT and TD(C)DFT. In the self-consistent calculation, linear interpolation is used for the communication between the numerical solutions of the Maxwell equations and Schrödinger equations obtained on two different scale meshes. Figure 1 shows some numerical results. (see [4, 3] for more model calculations.)

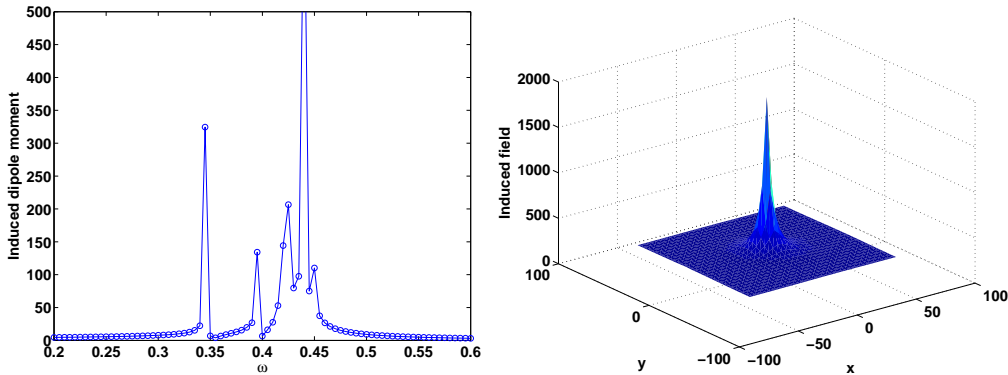


Figure 1: Methane ( $CH_4$ ): Left: induced dipole moment with respect to frequencies; Right: intensity of induced EM field at  $z = 0$  with lowest eigenfrequency  $\omega \approx 0.345$  (first peak of left figure). Units: a.u.

The proposed formulation reduces the computational cost of the semiclassical approaches greatly by incorporating the Density Functional Theory and the Time Dependent (Current) Density Functional Theory to handle the many-body Schrödinger equations. The multiscale scheme handles the different scales of the EM field and the matter (charged particles) well by allowing communications of the numerical solutions for the EM field and the density and/or current density from different mesh scales. Numerical examples show that resonant conditions can be obtained and resonant phenomenon is observed.

**Future projects:** For the multiscale scheme, the numerical solution of the macro solver does not need to be very accurate. In practice, we can either choose relatively low accuracy for the macro solver or dynamically increase the accuracy with respect to iterations for the macro solver starting from very low accuracy. In this way, the CPU time can be reduced. We will further investigate such a technique in ongoing projects.

We plan to utilize current approach to study more nanostructures, e.g. the self-assembly of quantum dots. In DFT and TD(C)DFT, the effective mass approximation will be used to carry out the self-consistent electronic structure calculation, then the coupled Maxwell-TD(C)DFT approach will be applied to study the optical property. We will mainly study the size dependence and the dependence of numbers of electrons for the resonant conditions. Particularly, we will work on the parallel implementation of current approach as the number of samples (quantum dots) increases. Further applications including the study of periodic nanostructures will be considered.



### 3 Computational High Frequency Wave Propagation

Finding efficient and accurate numerical solutions for the Helmholtz equation,

$$\nabla_{\mathbf{r}}^2 U + \frac{\omega^2}{v^2} U = -\delta(\mathbf{r} - \mathbf{r}_0), \quad (2)$$

with  $\mathbf{r}_0$  being the source point,  $\omega$  the frequency, and  $v(\mathbf{r})$  the velocity field, is highly desirable in many important fields, e.g. acoustics, elasticity, electromagnetics, quantum mechanics and geophysics. There are mainly three classes of methods [13, 14]: (1) direct discretization of the Helmholtz equation and iterative solutions of the resulting linear system; (2) boundary integral or volumetric integral representations of the wavefield; and (3) geometrical optics type asymptotic expansions of the wavefield when the frequency is high.

Within the high frequency regime, a direct solver may not be feasible because a discretization that resolves the wavelength will result in a system that requires huge demand for both storage and computation power; the boundary integral representation of the wavefield provides an efficient way but mostly only applicable for cases in homogeneous media because analytical Green function is needed.

#### 3.1 Our approach: work in [27, 30]

We utilize the geometrical optics approach [13]. When the frequency  $\omega$  is high, one can assume that the wavefield  $U$  has the following geometrical-optics ansatz,

$$U(\mathbf{r}, \omega; \mathbf{r}_0) = A(\mathbf{r}; \mathbf{r}_0) e^{i\omega\tau(\mathbf{r}; \mathbf{r}_0)} + O\left(\frac{1}{\omega}\right), \quad (3)$$

where  $A$  is the amplitude and  $\tau$  is the phase function. Substituting (3) into (2), and collecting the terms of  $O\left(\frac{1}{\omega}\right)$ , one can find that  $\tau$  and  $A$ , respectively, satisfy the following eikonal equation,

$$|\nabla_{\mathbf{r}}\tau| = s(\mathbf{r}), \quad (4)$$

and the transport equation,

$$\nabla_{\mathbf{r}}\tau \cdot \nabla_{\mathbf{r}}A + \frac{1}{2}A\nabla_{\mathbf{r}}^2\tau = 0, \quad (5)$$

where  $s = 1/v$  is the slowness field. Since both the amplitude  $A$  and the phase  $\tau$  do not depend on frequency  $\omega$ , one can first compute the phase function  $\tau$  efficiently through (4), then the amplitude  $A$  through (5), and finally reconstruct  $U$  with the ansatz (3) faithfully in the region before caustics appear.

One of the challenges for solving (4) and (5) is that  $\tau$  and  $A$  have strong upwind source singularities. As a consequence, any direct first order or high order finite difference solver can only have polluted first order accuracy and relatively large errors because the error at the source will spread out to the whole space. In order to compute high order accurate traveltime and amplitude to construct reliable wavefield, we utilize a factorization approach [16, 27, 30] to resolve the source singularities of the phase function  $\tau$  and the amplitude  $A$ . For the factorization approach, the traveltime (amplitude) is decomposed into two factors, one of which is the traveltime (amplitude) corresponding to homogeneous media. Hence it is known analytically and captures the source singularity, which leaves the other factor smooth at the source. We then apply a high order WENO based Lax-Friedrichs scheme to compute the other factor, hence reliable traveltime and amplitude and be obtained to construct wavefield. The wavefield constructed with our approach approximates the true wavefield faithfully before caustics appear (see [27, 30] for numerical experiments).

#### 3.2 Beyond geometrical optics: work in [28]

When the caustics appear, the geometrical-optics ansatz is no longer valid because the amplitude is unbounded [13]. In order to obtain  $U$  even when the caustics appear, we propose to incorporate the Huygens principle into the geometrical-optics approximation. For each point  $\mathbf{r}$  in an interested observation region  $\Omega$ , the field at this point can be constructed through the Huygens-Kirchhoff integral [2, 33],

$$U(\mathbf{r}; \mathbf{r}_0) = \int_{\mathcal{S}} G(\mathbf{r}'; \mathbf{r}) \nabla_{\mathbf{r}'} U(\mathbf{r}'; \mathbf{r}_0) \cdot \vec{\mathbf{n}} - U(\mathbf{r}'; \mathbf{r}_0) \nabla_{\mathbf{r}'} G(\mathbf{r}'; \mathbf{r}) \cdot \vec{\mathbf{n}} dS, \quad (6)$$

where  $\mathcal{S} \ni \mathbf{r}'$  is the closed surface enclosing the domain, and  $G(\mathbf{r}'; \mathbf{r})$  is the Green function satisfying the Helmholtz equation (2) with point source  $\mathbf{r}$ . For inhomogeneous media, our geometrical optics approach

above provides an efficient way to construct the Green function  $G$ , hence the Huygens-Kirchhoff integral can be evaluated.

The high cost of computing the Green function  $G$  for all source points  $\mathbf{r}$  in the observation region  $\Omega$  is further resolved by exploring the reciprocal relations for the amplitude  $A$  and the traveltime  $\tau$ , i.e.  $A(\mathbf{r}'; \mathbf{r}) = A(\mathbf{r}; \mathbf{r}')$  and  $\tau(\mathbf{r}'; \mathbf{r}) = \tau(\mathbf{r}; \mathbf{r}')$ , hence for the Green function  $G$ . Therefore only traveltimes and amplitudes corresponding to secondary sources on the boundary  $\mathcal{S}$  are computed. Note that since they are independent of frequency, they are computed once and stored for reconstruction of wavefield of a band of high frequencies. Our Huygens principle based geometrical optics approach is the follows,

- The domain is decomposed into subdomains (layers), for each layer, the geometrical optics ansatz is valid. In some sense, we simulate the Huygens principle for wave propagation.
- For secondary sources on  $\mathcal{S}$ , computing the tables of traveltime, amplitude and takeoff angle, which is done on a coarser mesh. These tables are stored (on hard drive) and can be used to construct wavefield for any high frequencies.
  - Given frequency  $\omega$ , the tables of traveltime, amplitude and takeoff angle are loaded from hard drive to construct the wavefield. For each table, the data is interpolated onto a finer mesh first, and then the Huygens-Kirchhoff integral is computed. The tables can be loaded one by one so that the memory storage is low.

The wavefield constructed with our approach approximates the true wavefield faithfully when caustics appear. Figure 2 shows some numerical results. (see [27, 30] for more numerical experiments.)

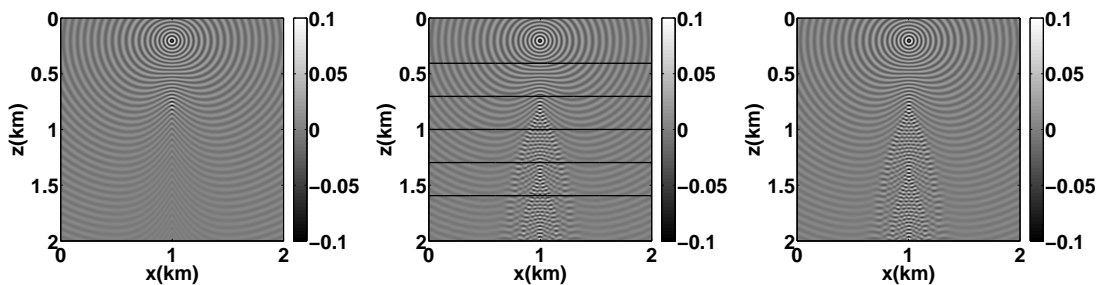


Figure 2: Wavefield of Waveguide model with frequency  $\omega = 32\pi$ . Left: constructed with first arrivals with geometrical optics; Middle: constructed with combined geometrical optics and Huygens-Kirchhoff integral; Right: computed by a direct 9-point Helmholtz solver. Solid lines are the lines of secondary sources.

**Future projects:** Since the tables of traveltime, amplitude and takeoff angle must be precomputed and stored on hard drive for reconstruction of wavefield. Data compression will be necessary especially in 3-D cases. Currently, we are working on data compression with Chebyshev polynomial expansions, which will be good enough for the migration and save storage for the data. More importantly, we are working on fast evaluation of the Huygens-Kirchhoff integral. The approach we are working on is the fast multidirectional method which is applicable due to the data compression with Chebyshev polynomial expansions that provides a low-rank separation of the Green function. Our approach is different. Instead of using multidirections, our approach will be applied dimension by dimension so that there is no need to use data structure like quadtree or octree.

Future projects include,

- Geometrical optics approach for Maxwell equations in high frequency regime.
- The combined Huygens principle and geometrical optics approach for reflection, diffraction and scattering problems.
- Inverse problems in geophysics/seismology.

## 4 Numerical Methods for Hamilton-Jacobi Equations

The Hamilton-Jacobi equation (HJ) with Dirichlet boundary conditions has wide applications on classical mechanics, geophysics, computer visions, optimal control and etc. Due to the nonlinearity, classical solutions

do not exist in general. The theory of viscosity solutions introduced by Crandall and Lions [12] has been applied successfully to study (HJ) both in theory and in practice. Our work mainly focus on monotone upwind schemes, e.g. the fast sweeping method [40, 8, 47, 37], for efficiently computing the viscosity solutions. The convergence of the fast sweeping method can be proved either by its monotonicity and consistency [5] or by proving its equivalence to the Hopf formula [20] as in [32]. The fast convergence is demonstrated by a contraction property in [32], where a formal error estimate is also given. When there is source singularity, it is at most  $O(|h \log h|)$  for both first order and higher order finite difference methods, since the source singularity is upwind and the error at the source will spread out to the whole space.

#### 4.1 Factored singularity: work in [16, 29]

In order to resolve the source singularities, we propose to use a factorization approach which has much lower computational burden compared with the adaptive gridding method [36] and does not need to assume homogeneity around the source, as in e.g. [42, 46, 7].

The factorization approach decomposes the traveltime into two factors,

$$\begin{cases} \text{Multiplicative factors: } \tau = \tau_0 u, \\ \text{or} \\ \text{Additive factors: } \tau = \tau_0 + u, \end{cases} \quad (7)$$

$\tau_0$  is the traveltime in homogeneous media, hence it is known analytically and captures the source singularity. As a result, the other factor  $u$  is differentiable at the source and satisfies a factored equation, which can be easily solved with  $O(h)$  accuracy ([16, 29]). Hence the traveltime can be recovered with  $O(h)$  accuracy.

#### 4.2 Applications

We have successfully applied the fast sweeping method with the factorization approach to numerically compute continuous traffic congestion equilibria [26], where an adjoint state method is designed for solving the variational problem modeling the traffic congestion,

$$(\mathcal{P}^*) \quad \inf \{ \mathcal{J}(\xi) : \xi \in L^{q^*}, \xi \geq \xi_0 \}, \quad (8)$$

with

$$\mathcal{J}(\xi) = \int_{\Omega} H^*(x, \xi(x)) dx - \int_{\bar{\Omega} \times \bar{\Omega}} \tau_{\xi}(x, y) d\gamma(x, y), \quad (9)$$

where  $\tau_{\xi}$  is the geodesic distance with respect to metric  $\xi$ ,  $\gamma$  models the transportation plan and  $H^*(x, \xi)$  models the congestion cost. For the adjoint state method, the forward equation and the adjoint state equation are solved by the fast sweeping method with/without the factorization approach. Figure 3 shows some numerical results.

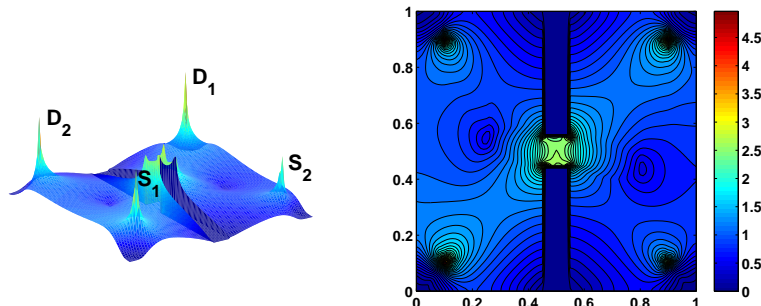


Figure 3: The equilibrium metric of a two-Source two-Destination model with a river running through the city. A bridge over the river connects the two sides of the city. Left: surf plot; Right: contour plot.

We have also applied the fast sweeping method in computer vision by designing an efficient scheme to compute the Euclidean skeleton of an object directly from a point cloud representation on an underlying grid [25]. The main ingredient of the scheme is the closest points information from the boundary, which is computed with the fast sweeping method efficiently. Figure 4 shows some numerical results.

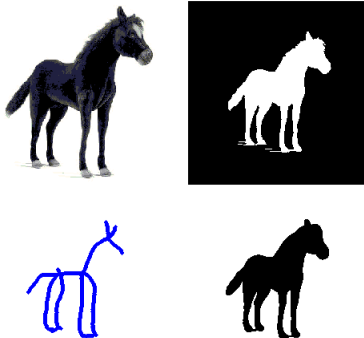


Figure 4: The skeleton of a model horse (bottom left) and reconstruction of the horse (bottom right).

**Future projects:** Currently, we are working on an adjoint state method for the attenuation X-ray transform, aiming to recover both the source and the attenuation at the same time. The fast sweeping method is used to solve both the forward and the adjoint state equations.

We plan to apply our method, with or without factorization, to numerical study the X-ray transform tomography and inverse geodesic X-ray transform (see [35] and reference therein). The fast sweeping method will be applied to solve the forward equation related to the geodesics, and possibly the Liouville equations and Fredholm type integral equations involved in the inversion formula.

### 4.3 Homogenization of Hamilton-Jacobi equations: work in [31]

Lions, Papanicolaou and Varadhan’s work on the following Homogenization problem [24]

$$(HJ) \begin{cases} u_t^\epsilon + H(Du^\epsilon, \frac{x}{\epsilon}) = 0, \\ u^\epsilon(x, 0) = g(x), \end{cases} \longrightarrow (HJE) \begin{cases} u_t + \bar{H}(Du) = 0, \\ u(x, 0) = g(x). \end{cases} \quad \text{uniformly as } \epsilon \longrightarrow 0, \quad (10)$$

has raised a lot of interests on computing the effective Hamiltonian  $\bar{H}(p)$ , e.g., (1) one can compute the homogenized solution from (HJE) without the need to resolve the small scale  $\epsilon$  if the  $x$ -independent  $\bar{H}$  is known; and (2) a program has been launched recently to use nonlinear PDEs to investigate some integrable structures within a dynamical system. And  $\bar{H}$  encodes a lot of dynamical information [15].

Existing algorithms to compute the effective Hamiltonian, for example the small- $\delta$  method, the large- $T$  method [38] and variational method [18], either require the solution of a cell problem for each  $p$  or require an extensive computation. Oberman, Takei and Vladimirovsky [34] proposed an idea to approximate  $\bar{H}$  when the Hamiltonian is convex and homogeneous of degree one in the gradient variable. Their basic idea is to recover the effective Hamiltonian from a suitable effective equation. The main advantage of this method is that only one auxiliary equation needs to be solved to approximate the effective Hamiltonian for all  $p \in \mathbb{R}^n$ . However, the assumptions on the Hamiltonian  $H$  is too restricted to include many other cases.

#### 4.3.1 Our approach

In [31], we propose a new formulation to compute effective Hamiltonians  $\bar{H}$  with the convex kinetic Hamiltonian

$$H(p, x) = \sum_{1 \leq i, j \leq n} a_{i,j}(x) p_i p_j + V(x), \quad (11)$$

and the convective Hamiltonian

$$H(p, x) = \frac{1}{2}|p|^2 + b(x) \cdot p.$$

Our formulation utilizes an observation made by Barron-Jensen [6] about viscosity supersolutions of Hamilton-Jacobi equations such that the inequality in the definition is in fact an equality when the Hamiltonian is convex. As a consequence, we can relate the effective Hamiltonian to a suitably chosen effective equation. The main advantage of our formulation is that only one auxiliary equation needs to be solved in order to compute the effective Hamiltonian  $\bar{H}(p)$  for all  $p$ . Both rigorous theoretical and numerical results including error estimates are presented to verify our formulations. Figure 5 shows some numerical results.

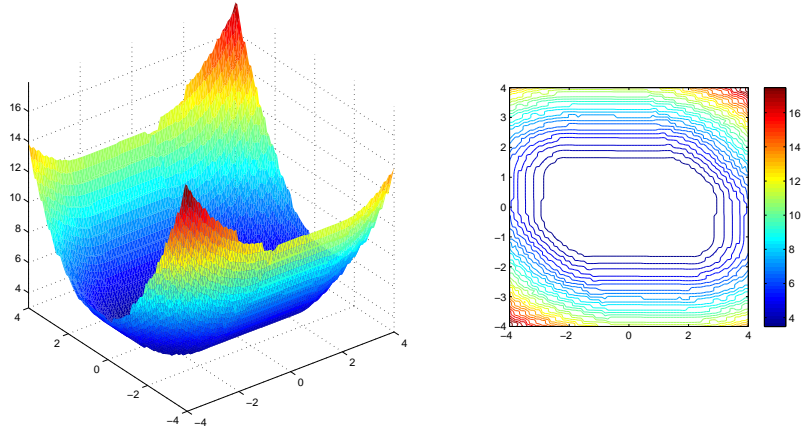


Figure 5: The computed effective Hamiltonian of a double pendulum model. Left: surf plot; Right: contour plot.

**Future projects:** (1), we are working on a proof to show  $O(\epsilon)$  error estimate for high dimension; (2), we are working on a fast scheme to solve effective Hamilton-Jacobi equations after  $\bar{H}$  is obtained; and (3), we plan to extend our method to deal with convex but noncoercive Hamiltonians, for example, the G-equation  $G_t + |DG| + b(x) \cdot DG = 0$ . The convective Hamiltonian  $H(p, x) = |p| + b(x) \cdot p$  is convex but not coercive when the velocity field  $b$  is too large. The corresponding effective Hamiltonian has been used in the combustion theory to model the *turbulent flame speed* [39].

## 5 Others

Besides the ongoing and future projects outlined above, once the approaches proposed above are mature, we plan to study a series inverse problems in electromagnetics and high frequency wave propagation.

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# Teaching Statement

Songting Luo \*  
Department of Mathematics  
Michigan State University

The goal of teachers in a mathematics class is not just indoctrination, but also teaching a way of analyzing and thinking. And the students want both knowledge and the ability of reasoning. Since teachers and students have the same goal, now the question is "how will a teacher achieve this goal in a mathematics class?"

In order to let the students absorb what we teach in a class, the first requirement is a clear lecture. Secondly, how to be interactive between teachers and students is very important. The atmosphere we create and the effort we make to view mathematics through students' eyes should be considered. We may expect the students to discover the joy of learning mathematics for themselves, but we should be sensitive to their backgrounds and limitations. Therefore, in a mathematics class, we will not make the lecture either too easy or too difficult. A too easy lecture will leave them without curiosities, while a too difficult lecture will make them frustrated. Asking students questions in a class according to such rules is always a good way to get students involved in our lecture, making them excited and willing to learn. A lecture should let students feel fun and motivated. For both lower-level or upper-level courses, instead of just following the textbook and writing down equations or formulas, we should try to explain the backgrounds or physical meanings of the equations and formulas. In such a way, the students not only be able to memorize the formulas and equations, but also can understand them, use them and keep them in mind for a long time.

Outside the classroom, we should be available to students when they have questions or curiosities about mathematics. Necessary assistance will help students improve a lot.

At the Michigan State University, I have taught Calculus and an advanced course on Mathematical Finance in last few semesters. For the Calculus course, I gave lectures with chalks and blackboard, assigned homework assignments after every lecture, took homework-based quizzes and regular exams. For the course on Mathematical Finance, I followed the suggestion from the course coordinator, gave lectures with projected slides, assigned homework assignments after every lecture, and took regular exams. It turned out that lectures with chalks and blackboard were more effective to attract the students' attention and let them involved, mainly because the pace of using chalks and blackboard is similar to the pace that students assimilate new ideas. Nevertheless, I am trying to find an optimal way to blend new and old technologies in a classroom.

I am interested in teaching both undergraduate and graduate courses, including different levels of Calculus, Linear Algebra, Numerical Linear Algebra, Numerical Differential Equations, Numerical Analysis and Numerical Partial Differential Equations and so on. My research background on computational and applied mathematics will be helpful for the students.

In conclusion, teaching mathematics is not just passing what we have learned or we know into students' mind, but also teaching students how to think in a mathematical way. We should help students improve both their knowledge and ability of analyzing from a mathematics class in better ways. And I am willing to be this teacher.

---

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**MICHIGAN STATE**  
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October 30, 2011

Dear Colleagues:

It is a great pleasure to recommend Dr. Songting Luo for a tenure-track Assistant Professor position. Songting is a dedicated young mathematician with substantial research potential.

I have known Songting since he was a graduate student at University of California in Irvine. His PhD thesis supervised by Professor Hongkia Zhao on fast and accurate numerical solution of the Hamilton-Jacobi equations addressed some key issues for the class of important problems with many applications in wave propagation. In my view, the thesis and their subsequent research as well as journal publications [1-9] represent the state of the art for the important research area.

After completing his PhD degree in 2009, Songting accepted our very first MCIAM postdoc position and has broadened his research scope by collaborating with several of us here at MSU. In fact, as a policy, our Center postdocs are encouraged to talk to all of the affiliated faculty members. In particular, Songting has been instrumental in our NSF FRG group effort on the modeling, analysis, and computation of nano optics, an emerging area in applied math that holds promises for substantial potential impact on nanotechnology and biotechnology. Because of the small scale features, the most viable detection or measurement method is via optics. Although significant advances have been made in experiments of the interactions between light and nano-scaled materials/structures, rigorous mathematical modeling presently is completely open. In nano optics modeling, the fundamental challenge is the mismatch of the scales. In other words, the model problem is not only large scale, but also by default of multi-scale. In order to solve the problem, it is essential to develop novel multiscale methods. In addition, the PDE models become more complicated since the classical Maxwell equations are not longer adequate in the nano scale, which offers significant research opportunities in mathematical analysis of PDEs. Due to the significance of the area, I led an effort of a research group consisting of researchers from MSU, Stanford, and Lawrence Berkeley National Lab to develop a Focused Research Group proposal which was funded by NSF in 2010. Songting participated in the effort from the beginning. Along with my colleague Di Liu and myself, Songting begun to investigate the linear optical responses of a nano medium. By developing a semi-classical approach, the model problem may be reduced to a coupled Maxwell-Schrodinger equation model. Essentially, Maxwell's equations are used for modeling the large scale features; while the small scale features are captured by the Schrodinger equations. Computationally, the Density Function Theory (DFT) method, a crucial model reduction method, has to be employed for the solving the many body Schrodinger equation. Songting has been the main contributor of the project and been fully responsible for the computational models and algorithms. The initial research



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findings [10-11] are very promising which shed some light on this original and significant project. In addition to working with Di Liu and myself, Songting has also collaborated with my colleagues Jianliang Qian at MSU on topics related to his thesis project.

Through the projects, Songting has clearly demonstrated a well blended set of skills in analysis, computation, and his solid background in applied mathematics. His broad knowledge in physics is impressive. All of the projects mentioned above are of long term nature with significant number of important open problems. Let me also add that Songting's publication record is simply outstanding at this stage of his career. In addition, it is highly likely that Songting will continue to produce high quality work in the field.

As the main mentor at MSU, I was also asked to comment on Songting's teaching performance. Since his arrival in 2009, Songting has taught four undergraduate classes in calculus and math finance. In fact, I visited his Calculus class a few times during the period. Based on my own observations, Songting really came across as a knowledgeable teacher who cares about his students. His presentations including those for his conference talks are always well organized.

On the personal level, Songting is a pleasant person with a fine sense of humor.

In summary, Songting Luo has demonstrated creativity and originality through his research. He is committed to scientific research in applied and computational mathematics at the high level and will be a valuable addition to any top applied/computational mathematics program.

I enthusiastically support his application. Please feel free to contact me if additional information is needed.

Sincerely yours,

A handwritten signature in cursive script that reads "Gang Bao".

Gang Bao  
Professor and Director  
Michigan Center for Industrial and Applied Mathematics  
Department of Mathematics  
Michigan State University  
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# Reference letter for Songting Luo

Jean-David Benamou \*

23 novembre 2011

## To whom it may concern,

I met Songting Luo during summer 2006 while visiting Professor Hongkai Zhao at UC Irvine. We then started a research collaboration on a new second order scheme for the Eikonal equation. The collaboration extended over academic year 2007/2008 and Songting visited several times Rice University where I was visiting Professor. It has been a fruitfull collaboration and we published a paper. Songting was very much involved in this research, in particular he diagnosed and fixed a serious flaw in the first version of the scheme. At that time he was a PhD student and my work experience with him was extremely enjoyable. I remember Songting as a very good mathematician with excellent programming skills. He is rigorous and careful. He picks up new ideas easily but also brings his own original contributions to the discussion. He definitely is a hard worker.

I took the time to read Songting vita, research statement and several of his last pre-prints in order to provide a fresh and up to date opinion on his work.

Let me first say that this reading did more than confirm my very good opinion of Songting. I am impressed by the quantity and the quality of his work at MSU.

He already has seven publications, several in first class journals, and roughly the same number of papers submitted or preprints. He obviously has been a precious collaborator at MSU as he cosigned with different people. He also managed to keep his collaboration with Professor Zhao rolling.

Songting still has a large activity in the Hamilton-Jacobi/ High Frequency wave propagation numerical field but has also expanded his research in several new directions. Most notably, I think the paper on nano optical response with G. Bao and D. Liu is first class. It seems that Songting activity has significantly drifted towards multiscale/homogenization problems (the paper on Effective Hamiltonians with HK. Zhao is excellent) and this is good news as these are important topics and we need good numericians there.

In summary, I strongly support Songting desire to pursue an academic career in applied mathematics. He is more than ready to get a more stable and independant position.

---

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Dear Colleague:

It is really my great pleasure to recommend Dr. Songting Luo for a tenure track position in your department. Songting is finishing his third year postdoc at MSU. During his stay, he has been working with me and G. Bao on a very interesting while challenging project on nano-optics. Through interactions we had, he has impressed me as a highly dedicated young researcher with a very broad skill set. I believe he will be a very good fit for any top tier math department.

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As the technologies on nano-scale advance, mathematical modeling and computational tools are becoming more important in understanding complex physical processes. New challenges arise when investigating nano-scale phenomena, which will involve multiple scales of Physics, as well as corresponding efficient numerical schemes. This is very well illustrated by the example of nano-optics. As the size of nano-optical devices get smaller, the optical response of the materials exhibits more nonlocal and nonlinear effects that are quantum mechanical in nature. Well established Physics describing the system is the Quantum Electrodynamics (QED), which has the disadvantage of numerical intractability. The so called semi-classical theory treats the electromagnetic fields classically with Maxwell equations and the motion of charged particles quantum mechanically with Schrödinger equations. This greatly simplifies the model, but still need poses great numerical challenges for the high dimensional coupled system.

The idea we had, is to couple efficient solvers for Maxwell equations with Time Dependent Density Functional Theory (TDDFT) for excited states of the electronic structures. TDDFT solves the electron density, instead of the wavefunction, of the electronic system, which is able to reduce the dimension

of the problem from  $3N$  to  $3$ . A multi-scale scheme is needed to solve the coupled Maxwell+TDDFT equations. As expected, this is a very challenging project for a junior person like Songting. He tackled the problem head on. With great efforts, he quickly caught up the Physics background and got the base ideas of TDDFT . He has successfully formulated a system of equations in the regime of linear response and designed a multiscale iterative methods to efficiently solve it. The method has been applied to the study of Near Field Optics for anon-structures. We have two papers submitted to SIAM Multiscale Moldeing and Simulation and Optics Express.

During our group meetings and workshops I organized, Songing has given nice presentations. I have no doubt about his teaching skills. Reading his student evaluations, I found how his students love him. Here are some quotes from the students comments: *'He is a good instructor who is willing to help'*. *'He is awesome, very understanding'*. *'Luo is very understanding of students who struggle not only with the math but also the language behaviour. He works with the class because he does not like students getting bad grades.'* He is able to achieve above average scores in these evaluations.

In short, I found Dr. Luo to be a well driven researcher who can stand up to any difficulty. And he has been well trained for research in scientific computing. He also has sufficient communication skills and the right personality to work with. I think he will be a very constructive member for any math department that has high standards on research and teaching.

Sincerely,

Di Liu  
Associate Professor of Mathematics

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*MSU is an affirmative-action,  
equal opportunity employer.*

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Sincerely,

Di Liu  
Associate Professor of Mathematics

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October 25, 2011

**Letter of Recommendation for Songting Luo**

Dear Colleague,

It is my greatest pleasure to write a letter of recommendation for Songting Luo who has applied for a tenure track position at your university. I know him very well since he has been a visiting assistant professor in our department and our Michigan Center for Industrial and Applied Mathematics (MCIAM) since September 2009. I have an extremely high opinion of Luo's research achievements and research potential. His work combines mathematical theory, numerical analysis, and scientific computing. He is an absolutely first-rate hire for any department interested in cutting edge modern applied mathematics research and scientific computing.

His research works involve fast algorithms for nonlinear Hamilton-Jacobi equations, numerical homogenization for Hamilton-Jacobi equations, computational Eulerian geometrical optics, and related applications in nano-optics. Hamilton-Jacobi equation arises in many applications such as geometrical optics, crystal growth, etching, computer vision, obstacle navigation, path planning, photolithography, and seismology. Next I give a detailed summary of his research achievements.

First Songting Luo arrived to begin his postdoc training in September 2009 with a strong mathematical background from the University of California at Irvine in fast algorithms for Hamilton-Jacobi equation and numerical Homogenization (see Luo et al 2009; Luo et al 2010; Luo et al 2011; Luo et al 2011). He already had strong training for developing novel algorithmic ideas combined with the ability to perform difficult simulations on a suite of complex applications.

In his post doc work with me since September 2009, we have been developing a new mathematical framework for computing high frequency waves beyond caustics by utilizing some newly developed fast algorithms for computational Eulerian geometrical optics. This framework involves combining fast sweeping methods for eikonal and transport equations with some novel integral identity. Many new mathematical issues arise due to the extremely high-frequency waves and caustics-induced multi-scale phenomena that need to be resolved. We already have three formally accepted papers on these topics and one undergoing second-round review; of course, two more are already in the pipeline. Because these works are extremely important for many applications, please allow me to tell you more about Songting's works.

Let me start with his paper titled **"An Adjoint State Method for Numerical Approximation of Continuous Traffic Congestion Equilibria"** published in *Communications in Computational Physics*. In this work, Songt-



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ing proposed a novel adjoint state method and designed related fast algorithms for computing continuous traffic congestion equilibria. In traffic flow for transportation and communication, network equilibrium models are commonly used for prediction of traffic patterns in transportation and communication networks that are subject to congestion. In a recent work by G. Carlier, C. Jimenez, and F. Santambrogio (SIAM J Optimal Control 2008), they introduced a continuous version of Wardrop’s equilibria, proved the existence of continuous traffic congestion equilibrium by introducing a variational problem analogous to the discrete convex programming by Beckman et al (1956), and related it to the optimal transportation problem with congestion. It turns out that such an equilibrium is linked to a certain metric, and all actually used paths (the continuous version of routes) must be geodesics for this metric. Moreover, Benmansour et al (Netw. Heterog. Media 2009) have shown that an equilibrium metric is the solution of a variational problem involving geodesic distances. To solve this particular variational problem, Benmansour et al (Numer. Math. 2010) have designed a subgradient marching method to approximate continuous traffic congestion equilibria, and this method requires intensive memory and is computationally inefficient.

Therefore, Songting proposed an adjoint state method to numerically approximate continuous traffic congestion equilibria through the continuous formulation. The method formally derives an adjoint state equation to compute the gradient descent direction so as to minimize a nonlinear functional involving the equilibrium metric and the resulting geodesic distances. This gradient is proved to yield a descent direction, thus the resulting method is convergent. The geodesic distance needed for the state equation is computed by solving a factored eikonal equation, and the adjoint state equation is solved by a fast sweeping method.

Numerical examples demonstrate that the proposed adjoint state method produces desired equilibrium metrics and outperforms the subgradient marching method for computing such equilibrium metrics. On a given mesh with  $N$  grid points, for the subgradient marching method, the complexity of the fast marching method for solving the eikonal equation is  $O(N \log N)$  with the factor  $\log N$  as a result of the heap-sorting process; thus the computational cost for updating the subgradient at each grid point is  $O(N \log N)$ . Since one needs to update the subgradient at  $N$  grid points, the total complexity is  $O(N^2 \log N)$  (Benmansour et al (Numer. Math. 2010)); the updated metric and the subgradient at each grid point need to be stored to carry out each iteration; the former requires  $O(N)$  memory space and the latter requires  $O(N^2)$  memory space; thus, the total memory requirement is  $O(N^2)$ . For the adjoint state method, the fast sweeping method for both the factored eikonal equation and the adjoint state equation is of computational complexity  $O(N)$ ; therefore the total computational complexity is  $O(N)$ ; the adjoint state and the updated metric need to be stored to carry out each iteration, and the memory requirement is  $O(N)$ . Consequently, our **fast-sweeping based adjoint state** method is **one-order**

**faster than the subgradient marching** method in terms of **computation** and is **one-order more efficient than the subgradient marching** method in terms of **memory**.

In his paper titled “**Fast sweeping methods for factored anisotropic eikonal equations: multiplicative and additive factors**” (to appear in *Journal for Scientific Computing*), he proposed two novel fast sweeping methods for anisotropic eikonal equations with point source singularity. The viscosity solution of static Hamilton-Jacobi equations with a point-source condition has an upwind singularity at the source, which makes all formally high-order finite-difference scheme exhibit first-order convergence and relatively large errors. To obtain designed high-order accuracy, one needs to treat this source singularity during computation. In this paper, he applies the factorization idea to numerically compute viscosity solutions of anisotropic eikonal equations with a point-source condition. The idea is to factor the unknown traveltime function into two functions, either additively or multiplicatively. One of these two functions is specified to capture the source singularity so that the other function is differentiable in a neighborhood of the source. Then he designed monotone fast sweeping schemes to solve the resulting factored anisotropic eikonal equation. The resulting monotone schemes for 2-D and 3-D examples indeed yield clean first-order convergence rather than polluted first-order convergence and both factorizations are able to treat the source singularity successfully.

To put this result into a broad viewpoint, let me emphasize that **some other algorithms for anisotropic eikonal** equations in the market are very troublesome to implement even in 2-D cases, **not even to mention 3-D cases**, while our fast-sweeping based methods can be **easily implemented in both 2-D and 3-D cases**.

In his paper titled “**Factored singularities and high-order Lax-Friedrichs sweeping schemes for point-source traveltimes and amplitudes**” published in *JCP* (2011), he developed novel fast higher-order methods for computing traveltimes and amplitudes with point-source singularity. In the high frequency regime, the geometrical-optics approximation for the Helmholtz equation with a point source results in an eikonal equation for traveltime and a transport equation for amplitude. Because the point-source traveltime field has an upwind singularity at the source point, all formally high-order finite-difference eikonal solvers exhibit first-order convergence and relatively large errors. In this paper, he first proposed to factor out the singularities of traveltimes, takeoff angles, and amplitudes, and then he designed high-order Lax-Friedrichs sweeping schemes for point-source traveltimes, takeoff angles, and amplitudes. **These higher-order traveltimes and amplitudes can be used for constructing high-frequency wave fields for a broad band of frequencies in both 2-D and 3-D cases**. However, there is a catch that the resulting wave field is only valid before kinks appear in the single-valued traveltime field or caustics appear in the multivalued traveltime field. After kinks appear in the

single-valued traveltime field, the traveltime is no longer smooth so that the traditional geometrical optics ansatz is not valid any more.

Therefore, the challenge is to construct the wavefield in the high frequency regime beyond kinks in single-valued traveltime fields or caustics in multivalued traveltime fields. In the recent years, there is a lot of effort to develop multivalued eikonal solvers to compute multivalued traveltime field (Symes (1996); Engquist et al (2002); Osher et al (2002); Sethian et al (2002)); however, those approaches face the difficulty in constructing the high frequency wavefield itself because the Keller-Maslov index characterizing the phase shift associated with caustics is needed for the construction, and this index is hard to compute reliably when the ray structure related to the Hamiltonian system defined by the eikonal equation in inhomogeneous media is chaotic.

So here is Songting's **remarkable contribution**. Based on our work published in *JCP* 2011, he came up with a novel idea to go beyond caustics so that we are able to construct the high frequency wave field without using multivalued traveltimes explicitly. The new method has the following desired features: (1) it can automatically take care of caustics and incur no pollution errors; (2) it can construct Green functions of the Helmholtz equation for arbitrary wave numbers once a set of local traveltime and amplitude tables are computed. I have showed some computational results for the well-known Marmousi model to experts in geophysics, and they just like those figures. We are in the final stage to submit the paper to a top journal.

**In summary**, Songting Luo is a very talented, productive and creative modern applied mathematician working in central areas with large future growth potential involving fast algorithms for Hamilton-Jacobi equations, Eulerian computational geometrical optics for high frequency waves, and their applications. He already has significant research achievements and much more can be anticipated from him in the future. I rate him in the highest group of post-docs in the current job market. He will be a fantastic appointment for a tenure track applied math position at your university and I recommend him without any reservations!

Sincerely,

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**COMPUTATIONAL RESEARCH DIVISION**

Oct 15, 2011

To whom it may concern,

I am writing to recommend Dr. Songting Luo for a faculty or researcher position at your institute. I came to know Songting when I participated in a collaborative project headed by Professor Gang Bao at Michigan State university. Songting is a member of the project team. The goal of the project is to develop mathematical models and computational techniques for understanding nano-optics at multiple spatial and time scales. The approach we took is based on a semiclassical theory that couples the Maxwell equation with the Schrödinger's equation through current and charge densities. However, to understand the interaction of light with nanoscale materials that contain more than a few atoms, solving the Schrödinger equation itself is already computationally intractable. To overcome this difficulty, we replace the many-body Schrödinger's equation with a set of single-particle equations that are coupled by the charge density. These equations are defined by time-dependent (current) density functional theory (TD(C)DFT). Songting made significant contribution by deriving the coupling between the Maxwell and TDCDFT equations, and showed how these equations can be solved in a self-consistent fashion. He did not know much about density functional theory or quantum mechanics in general before he started to work on this project. But he was able to pick up the subject quickly and started making necessary changes to the existing DFT and TDDFT software package such as Octopus and KSSOLV. He did the code development and computational testing all by himself. He asked me many penetrating questions about the DFT theory and numerical algorithms. He even found and fixed a few bugs in the existing software. I was quite impressed that he was able to make a lot of progress within such a short period of time because, in my experience, the initial barrier for understanding DFT and its computation is usually quite high for computational mathematicians that do not have a fair amount of training in quantum mechanics. But this does not seem to be a problem for Songting. It shows how talented he is and how strong his mathematical skills are. His work resulted in a number of reports that will soon be submitted for publication. I think these papers will generate a lot of interest both in the mathematics and the physics communities.

What is even more amazing is that nano-optics is not the only project that Songting works on. Judging from his publication record, I believe he is highly productive in developing novel algorithms for solving wave propagation and Hamilton-Jacobian equations. Songting works extremely hard, and is always eager to learn new problems and develop new ideas. He has a solid background in numerical analysis and a good sense of how to apply theoretical results and numerical techniques to practical problems. He is very easy to work with and his communication skills are excellent. I am very confident that he will do well in his future scientific career.

Sincerely yours,

Chao Yang  
Staff Computer Scientist



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October 25, 2011

### **Recommendation Letter for Songting Luo**

I am writing to strongly support Songting Luo's application to your institute. He is my former Ph.D student and has been a postdoc at Michigan State University since he graduated in 2009. Songting is a talented and solid young applied and computational mathematician. As you can see from his productive research work, he can do both analysis and computation as well as modeling and applications. He is very hard working and motivated. In his thesis he studied efficient numerical methods for Hamilton-Jacobi equations, a class of nonlinear hyperbolic partial differential equation (PDE) which has important applications in geophysics, optimal control, image processing, computer vision, seismic imaging, etc. I am very satisfied with Songting's attitude, motivation, independence and effort in his research. He has made several significant contributions such as showing a contraction property of the fast sweeping method and its convergence, using factored eikonal equation to deal with source singularity, studying homogenization of a Hamilton-Jacobi equations using appropriate effective equation, and a few applications. As you can see this is a rather long list of achievements for a Ph.D thesis. After he graduated from UC Irvine, he went to the mathematics department at Michigan State University as a postdoc researcher. I am very happy to see that he has embarked in several very interesting projects and made significant progress in them in a relatively short period of two years. In particular their work on nano optical response using coupled Maxwell-Schrödinger multiscale formulation is very promising. I will leave to other experts in this field to address this work. Below I will comment on Songting's work on Hamilton-Jacobi equation and its applications in more detail.

Hamilton-Jacobi equations is a class of nonlinear hyperbolic PDE. Due to the nonlinearity of these equations global classical solution does not exist in general. An appropriate definition of weak solution, the viscosity solution is the right solution in many applications. Due to the nonlinearity of the PDE and possible singularities in the solution development and analysis of efficient numerical methods is of great importance.

Recently several efficient algorithms for solving static convex Hamilton-Jacobi equations, such as fast marching method (FMM) and fast sweeping method (FSM), have been proposed. Instead of marching in time they solve the discretized system of nonlinear equations directly according to the causality of the underlying PDE. Although monotone schemes is an important class of numerical schemes that guarantee the convergence of the numerical solution to the viscosity solution, upwind monotone scheme is absolutely crucial for the success of these fast methods. One of Songting's work is to study the contraction property of monotone upwind schemes and its implications on the fast convergence for iterative methods such as FSM. A particular interesting phenomenon is that the number of iteration may decrease when the mesh is refined which is totally different from common intuitions for elliptic equations. This is exactly because of the use of upwind scheme with proper ordering such that each update during the iteration contracts the error. So construction of upwind monotone scheme for general convex Hamiltonian is of great importance in practice. For convex Hamilton-Jacobi equations several discrete schemes have been proposed. Songting shows their equivalence, e.g., optimal control formulation based on Bellman's dynamical programming principle (Sethian and Vladimirsky, Bornemann and Rasch) and PDE formulation based on method of characteristics (Qian, Zhang and Zhao). The combination of these upwind monotone schemes with fast sweeping strategy provides extremely simple and efficient numerical methods especially for general convex Hamilton-Jacobi equation when using a fixed stencil may not be easy for Dijkstra type algorithms.

Songting, joint with Fomel and me, also developed a fast sweeping method for factored Eikonal equation. In many applications, such as in geophysics, point source singularity is commonly present and poses numerical difficulty such as loss of accuracy. Special treatments such as adaptive grid may be used to alleviate the problem. The factored Eikonal equation provides a nice and simple way to desingularize the original Eikonal equation at source point by decomposing the solution of a general Eikonal equation as the product of two factors: the first factor is the solution to a simple Eikonal equation which has similar type of singularity at the source, the second factor is a correction which is a smooth function. The factored Eikonal equation is posed on the correction. Our new method inherits the same efficiency of the fast sweeping method, i.e., a small number of iterations independent of mesh size, and improves the accuracy of the numerical solution significantly. Based on this work we are looking into slowness estimation in geophysics application. Recently Songting and his collaborators also extended this framework for more general anisotropic eikonal equations and improve both travel time and amplitude computation.

Another very nice piece of work of Songting, joint with my colleague Yu and me, is on homogenization of Hamilton-Jacobi equation. Although Lions, Papanicolaou and Varadhan's work more than twenty years ago give an elegant mathematical characterization of the effective Hamiltonian by defining a clean cell problem, the cell problem does not convey much constructive or geometric

information about the homogenized Hamiltonian except in very simple setup. Nor does it provide much insight on how to numerically compute the homogenized Hamiltonian efficiently and accurately. One reason is because the cell problem has a periodic boundary condition which means one has to solve a hyperbolic problem on a torus where characteristics have infinite length. So there is no beginning, i.e., boundary condition, for information to start along characteristics. Existing algorithms to compute the effective Hamiltonian, for example the small- $\delta$  method, or the large- $T$  method require the solution of a cell problem for each  $p$ . In our approach we utilized an observation made by Barron-Jensen about viscosity supersolutions of Hamilton-Jacobi equations such that the inequality in the definition is in fact an equality when the Hamiltonian is convex. As a consequence, we can relate the effective Hamiltonian to a suitably chosen effective equation. The main advantage of our formulation is that only one auxiliary equation needs to be solved in order to compute the effective Hamiltonian  $H(p)$  for all  $p$ . Moreover, the effective equation becomes a boundary value problem for which efficient numerical methods such as FMM and FSM are available. Both rigorous error estimates, convergence and stability results are developed in our work.

In addition to the above work, Songting has also worked on several other projects at the same time. With Benamou and me, we developed a compact second order scheme that can be used as a one sweep postprocessing procedure for any first order scheme. The main advantage is that the scheme is upwind and compact. The correction utilizes the PDE and has a concrete geometric meaning. Songting with Guibas and me developed an algorithm to compute Euclidean skeletons of objects presented by point clouds, which is an important problem for shape recognition/classification in computer vision. Our algorithm is efficient with robustness to noise. It uses closest point information which can be computed efficiently on an underlying grid by FSM. Combining closest point information and distance-ordered-homotopic thinning process we can identify the Euclidean skeleton.

Finally let me mention one interesting but challenging ongoing project of Songting on numerical method for Hamilton-Jacobi equations, superconvergence of monotone upwind schemes in numerical gradient. It has been tested that the numerical gradient has a first order accuracy up to shocks for first order upwind scheme on both rectangular and triangular meshes. This phenomenon has important implications in many applications such as in geometric optics, computing optimal path, etc, where gradient information is used. This is a very challenging problem since even the accuracy of the numerical solution itself is quite hard to analyze due to nonlinearity and singularity. However, he is making some nice progress for some simple cases. If there is any progress it would be quite significant.

In all the above work, Songting has played a vital role. He has strength in both analysis and

computation. He also picks up new things quickly. I envision him to become a successful and original researcher in the near future. I recommend him enthusiastically.

Sincerely,

A handwritten signature in black ink, appearing to read 'zhao hkz', written in a cursive style.

Hongkai Zhao  
Professor and Chair



## Ratings for Luo, Songting

Positions Applied (rAvg)	Rating	ShortList	Interview	Offer	NotConsider
NTT (5.0)	struther 5				
	aelabovs: R: A T: NE S: NE struther: <i>Sweeping methods for several physical systems. Multiscale optics. Little comment about teaching.</i>				