WPI Workshop "Quantum Dynamics and Uncertainty Quantification"

Schedule

Tuesday

10:00-11:30 Olof Runborg
Uncertainty Quantification for High Frequency Wave Propagation

14:15-15:00 Ludwig Gauckler*
NLS numerics

* are other relevant WPI activities

15:30-17:00 Mohammed Lemou
Averaging techniques and numerical methods for
a class of highly oscillatory transport equations

Wednesday

10:00-11:30 Shi Jin
Semiclassical computationl methods for oscillatory and uncertain
non-adiabatic quantum dynamics

14:00-15:30 Olivier Pinaud
Waves in random media and applications

Thursday

10:00-11:30 Francois Golse
A convergence rate estimate for the semiclassical limit with Lipschitz
continuous force field

14:00-14:45 Yong Zhang*
NLS numerics
* are other relevant WPI activities

Abstracts

Shi Jin (University of Wisconsin-Madison and Shanghai Jiao Tong University)

Title: Semiclassical computational methods for oscillatory and uncertain quantum dynamics with band-crossings

Abstract:

Band-crossing is a quantum dynamical behavior that contributes to important physics and chemistry phenomena such as quantum tunneling, Berry connection, charge transfer, chemical reaction etc. In this talk, we will discuss some recent works in developing semiclassical methods for band-crossing in surface hopping. For such systems we will also introduce an nonlinear geometric optics method based "asymptotic-preserving" method that is accurate uniformly for all wave numbers, including the problem with random uncertain band gaps.

Olivier Pinaud (Colorado State University)

Title: "Waves in random media and applications"

Abstract:

We will review some results concerning uncertainties in the derivation of kinetic equations from wave propagation in random media, that is modeled by a wave or a Schroedinger equation. Kinetic equations usually describe quadratic quantities in the wavefield such as the energy or wave-wave correlations, and can be used to solve some imaging problems in complex media.

Olof Runborg (Mathematik Institution, Stockholm)

Title: Uncertainty Quantification for High Frequency Wave Propagation

Abstract:

We consider the wave equation with highly oscillatory initial data, where there is uncertainty in the wave speed, initial phase and/or initial amplitude. To estimate quantities of interest (QoI) related to the solution u^ε and their statistics, we combine a high-frequency method based on Gaussian beams with sparse stochastic collocation. In the talk we will discuss how the rate of convergence for the stochastic collocation and the complexity of evaluating the QoI depend on the short wavelength ε. We find in particular that QoIs based on local averages of $\vert u^\varepsilon\vert ^2$ can give fast convergence rates, despite the fact that u^ε is highly oscillatory in both physical and stochastic space.

Mohammed Lemou

Title: "Averaging techniques and application to numerical methods for highly oscillatory Vlasov and Klein-Gordon models"

Abstract:

A brief description of averaging theory for
highly-oscillatory problems will be first presented with an emphasis on the so-called classical and stroboscopic averaging methods. Then I will present two general strategies to construct efficient numerical schemes for a class of highly oscillatory PDEs: the so-obtained numerical schemes have a uniform accuracy with respect to the frequency. Two applications will be considered: the Vlasov kinetic equation with strong magnetic field and the Klein-Gordon equation in the non-relativistic regime.

François Golse

Title: A convergence rate estimate for the semiclassical limit with Lipschitz continuous force field

Abstract:

We propose an explicit bound for the convergence rate in the semiclassical limit for the Schrödinger equation which holds for potentials with Lipschitz continuous gradient. This bound is based on an analogue of the Wasserstein metric used in optimal transportation, adapted to measuring the distance between a quantum and a classical density.