#### 典型量子体系对应的 Wigner 方程的高精度数值方法

#### 陈珍珠

#### 北京大学 1401110036@pku.edu.cn

Wigner 方程是量子力学在相空间中的统计描述,它无缝连接了经典力学与量子 力学而且直接提供了理论物理和实验物理的对比量. 类比 Boltzmann 方程, Wigner 方 程有相似的数学结构,利用这些结构可以定义 Wigner 方程的特征线并用 semi-Lagrange 方法进行求解,这是高维 Wigner 方程存在有效确定型数值方法的关键. 此外, 利用拟微分项的两种等价形式: 卷积形式和级数形式,可以有效地处理无界势场. 该报告 的主要内容就是利用 Wigner 方程的数学结构设计高精度的确定型数值方法来模拟典 型的量子体系,例如,双势阱的的量子隧穿和量子双缝干涉. 主要工作如下:

(a) 对于一维单体系统, 我们利用拟微分项的两种等价形式, 将无界势场分解成无界的多项式逼近部分和有界衰减部分, 然后分别用 Moyal 级数和卷积来处理. 利用多项式的 Moyal 展开是有限项求和以及 Poisson 求和公式离散卷积项, 我们得到一个高阶的偏微 分方程. 最后, 对于这个偏微分方程, 我们设计了一个保证质量和能量守恒的谱方法. 利 用这个方法我们模拟了不同双势阱下的量子隧穿.

(b) 量子双缝干涉现象是量子力学中最重要的问题, 双缝可以用一个二维的无界势场进 行模拟, 为了准确地抓住量子干涉条纹的信息, 我们发展了一个高精度的四阶算子分裂 格式. 利用算子分裂格式将方程分解成两个子问题, 其中一个是 (x, t) 方向的对流方程, 一个是只包含了拟微分项的发展方程. 对于对流方程我们给出了解析的行波解, 然后用 Chebyshev 多项式展开来计算非网格点上的函数值. 对于拟微分项, 利用 Wigner 函数 在 k 方向的平面波展开, 解析地给出了展开系数的表达式. 这样我们得到了一个不依赖 时间步长的高阶算子分裂格式. 利用该数值格式我们模拟了不同双缝下的量子干涉实验, 并给出了收敛阶分析以及干涉条纹的具体信息.

# Extension and analysis of the decoupled and positivity-preserving DDFV scheme for diffusion problems to the three-dimensional case 董倩楠

北京应用物理与计算数学研究所 dongqiannan17@gscaep.ac.cn

A decoupled and positivity-preserving discrete duality finite volume (DPPDDFV) scheme has been proposed for diffusion problems on general polygonal meshes. We focus on further extensions of the DPPDDFV scheme in two respects, one in the threedimensional case and the other in analysis results. We extend the DPPDDFV scheme for anisotropic diffusion problems on polyhedral meshes with star-shaped cells and planar faces. The finite volume equations for the vertex-centered unknowns are established from the ingenious combination of a geometric relationship with the construction of the cell matrix. The finite volume equations for cell centered-unknowns are obtained by using the two-point flux approximation (TPFA) method. To guarantee the positivity of the two categories of unknowns, a positive post-processing method for vertexcentered unknowns is introduced. The characteristics of the DPPDDFV scheme in the 2D case have been inherited by the 3D counterpart. First, compared with most existing nonlinear positivity preserving schemes, nonlinear iteration methods are not required for linear problems and the nonlinear solver can be selected unrestrictedly for nonlinear problems. Second, the two sets of FV equations are decoupled. Third, the local conservation is strictly (resp. conditionally) maintained on the primary (resp. dual) mesh. Under some weak geometric assumptions, the stability and error estimate results for the vertex-centered unknowns are obtained. Furthermore, by assuming the coercivity of the FV equations for the cell-centered unknowns, a first order H1 error estimate is obtained for the cellcentered unknowns through the analysis of residual errors.

## High-order entropy stable schemes for special relativistic hydrodynamics 段俊明

#### 北京大学 duanjm@pku.edu.cn

This talk will introduce the high-order accurate entropy stable finite difference schemes for special relativistic hydrodynamic equations. The schemes are built on the entropy conservative flux and the weighted essentially non-oscillatory (WENO) technique as well as explicit Runge-Kutta time discretization. The key is to technically construct the affordable entropy conservative flux of the semi-discrete second-order accurate entropy conservative schemes satisfying the semi-discrete entropy equality for the found convex entropy pair. As soon as the entropy conservative flux is derived, the dissipation term can be added to give the semi-discrete entropy stable schemes satisfying the semi-discrete entropy to the found convex entropy reconstruction for the scaled entropy variables and the high-order explicit Runge-Kutta time discretization are implemented to obtain the fully-discrete high-order entropy stable schemes. Several numerical tests are conducted to validate the accuracy

and the ability to capture discontinuities of our entropy stable schemes. This is a joint work with Prof. Huazhong Tang.

#### A Characteristic-featured Troubled-cell Indicator for Conservation Laws based on Artificial Neutral Networks 冯亦葳

#### 北京航空航天大学 fengyw@buaa.edu.cn

In this work, we use exact solutions of the one-dimensional Burgers equation to train an artifificial neural network (ANN) with one hidden layer as a shock wave detector. The expression of the ANN detector is then rewritten in a pratical form to reflflect admissible jump of eigenvalues. We show the working mechanism of the practical form is consistent with compressing or intersecting of characteristic curves. In addition, we prove there is indeed a discontinuity inside the cell detected by the practical form, and smooth extrema and large gradient regions are never marked. As a result, we apply the practical form to numerical schemes as a troubled-cell indicator with its easy extension to multi-dimensional conservation laws. Numerical results are present to demonstrate the robustness of the present indicator under Runge-Kutta Discontinuous Galerkin (RKDG) framework, its performance is generally compared to TVB-based indicators more efficiently and accurately.

#### Regularity of minmizers of singular energy functional for nematic liquid crystals in 3D 取志远 纽约大学 zg574@nyu.edu

In Landau-de Gennes theory, the local state of liquid crystal polymers is characterized by a 3\*3 symmetric traceless tensor Q and the energy functional consists of two parts: elastic energy and bulk energy. Motivated by Ball and Majumdar' s modification of Landau-de Gennes model (where the bulk energy is singular), we study a tensor-valued variational obstacle problem in a 3D domain with prescribed boundary data and showed the regularity of the minimizer. Under certain assumptions, especially on blow up profile of the singular functional, we prove higher regularity of Q, and show that the set on which Q touches the obstacle is either empty, or small with characterization of its Hausdorff dimension. We also prove boundary partial regularity of the energy minimizer.

## Arbitrary Lagrangian-Eulerian discontinuous Galerkin method for hyperbolic equations involving \$\delta\$-singularities

#### 洪雪

#### 中国科学技术大学 xuehong1@mail.ustc.edu.cn

In this paper, we develop and analyze an arbitrary Lagrangian-Eulerian discontinuous Galerkin (ALE-DG) method for solving one-dimensional hyperbolic equations involving \$\delta\$-singularities on moving meshes. The \$L^2\$ and negative norm error estimates are proven for the ALE-DG approximation. More precisely, when choosing the approximation space with piecewise \$k\$th degree polynomials, the convergence rate in \$L^2\$-norm for the scheme with the upwind numerical flux is \$(k+1)\$th order in the region apart from the singularities, the convergence rate in  $H^{-(k+1)}$  norm for the scheme with the monotone fluxes in the whole domain is \$k\$th order, the convergence rate in  $H^{-(k+2)}$  norm for the scheme with the upwind flux in the whole domain can achieve  $(k+\frac{1}{2})$  th order, and the convergence rate in  $H^{-}$ (k+1) (R\backslash R\_T)\$ norm for the scheme with the upwind flux is (2k+1)\$th order, where \$R\_T\$ is the pollution region at time \$T\$ due to the singularities. Moreover, numerically the \$(2k+1)\$th order accuracy for the post-processed solution in the smooth region can be obtained, which is produced by convolving the ALE-DG solution with a suitable kernel consisted of B-splines. Numerical examples are shown to demonstrate the accuracy and capability of the ALE-DG method for the hyperbolic equations involving \$\delta\$-singularity on moving meshes.

#### 半经典极限下 Schrodinger 方程的扩展 WKB 近似的误差分析 胡嘉顺 清华大学 hjs16@mails.tsinghua.edu.cn

扩展 WKB 近似是经典的 WKB 近似的一个推广,后者是求解波动方程的几何光学 方法的重要组成部分。WKB 近似简便易行,然而其应用受到焦散点的制约。为了解决 焦散点问题,Gassian beam 方法以及 Gaussian wavepacket 方法都是很好的选择。 这些方法的误差分析以及高阶推广方面的工作有很多。扩展 WKB 方法也可以很好的处 理焦散点问题。它的核心思想是在局部坐标系中使用 WKB 分析,然后再通过单位分解 来构建一个不依赖于局部坐标的 ansatz。本实报告重点介绍我们对于一阶扩展 WKB 应用到半经典 Schrodinger 方程上的 L2 误差分析的证明。由于我们考虑的是一般的线性 Schrodinger 形式的方程,因此我们选取了线性的 Kdv 方程作为我们的算例。算例验证了扩展 WKB 方法的 L2 下的一阶渐进精度。

#### Second order type methods for manifold optimization 户将

### 北京大学 jianghu@pku.edu.cn

Manifold optimization is ubiquitous in computational and applied mathematics, statistics, engineering, machine learning, physics, chemistry and etc. One of the main challenges usually is the non-convexity of the manifold constraints. By utilizing the geometry of manifold, a large class of constrained optimization problems can be viewed as unconstrained optimization problems on manifold. In this talk, I will present our recent second order type methods for manifold optimization.

#### 全正矩阵的研究现状与困难问题 李冰杰 浙江大学 727443158@gg.com

全正矩阵在组合优化中有广泛的应用。它被视为联系离散优化问题和连续优化问题的桥梁。在全正矩阵的研究中,有很多困难的公开问题,其中包括全正矩阵锥的几何特征,全正矩阵的判断,全正秩的估计和全正矩阵的分解。本次报告我将介绍这些问题的研究现状,和我们对这些问题的思考和看法。

### A Variational Convex Hull Algorithm 李凌丰

## 香港浸会大学 18481337@life.hkbu.edu.hk

Seeking the convex hull of an object is a very fundamental problem arising from various tasks. In this work, we propose two variational convex hull models using level set representation for 2-dimensional data. first one is an exact model, which can get the convex hull of one or multiple objects. In this model, the convex hull is characterized by the zero sublevel-set of a convex level set function, and the level set function is required to be non-positive at every given point. By minimizing the area of the zero sublevel-set, we can find the desired convex hull. The second one is intended to get convex hull of objects with outliers. Instead of requiring all the given points are included, this model penalizes the distance from each given point to the zero sublevel-set. Literature methods have difficulties to handle outliers. solve these models, we develop efficient numerical schemes using alternating direction methods of multipliers. Some numerical examples demonstrate the advantages of the proposed methods. The results confirm that our models work well for various images.

#### A Stochastic Trust Region Framework for Policy Optimization 李勇锋 北京大学 YongfengLi@pku.edu.cn

We propose a stochastic trust region method for deep reinforcement learning. The trust region subproblem is constructed with a surrogate function coherent to the total expected reward and a general distance constraint around the latest policy. The proposed algorithm tends to generate a monotonic improvement of the total expected reward and the global convergence is guaranteed under moderate assumptions. Comparisons with the state-of-the-art methods demonstrate the effectiveness and robustness of our method over robotic controls and game playings from OpenAI Gym.

#### Low-rank Matrix Optimization Using Polynomial-filtered Subspace Extraction 刘浩洋

北京大学 liuhaoyang@pku.edu.cn

In this paper, we study first-order methods on a large variety of low-rank matrix optimization problems, whose solutions only live in a low dimensional eigenspace. Traditional first-order methods depend on the eigenvalue decomposition at each iteration which takes most of the computation time. In order to reduce the cost, we propose an inexact algorithm framework based on a polynomial subspace extraction. The idea is to use an additional polynomial-filtered iteration to extract an approximated eigenspace, and project the iteration matrix on this subspace, followed by an optimization update. The accuracy of the extracted subspace can be controlled by the degree of the polynomial filters. This kind of subspace extraction also enjoys the warm start property: the subspace of the current iteration is refined from the previous one. Then this framework is instantiated into two algorithms: the polynomial-filtered proximal gradient method and the polynomial-filtered alternating direction method of multipliers.

We give a theoretical guarantee to the two algorithms that the polynomial degree is not necessarily very large. They share the same convergence speed as the corresponding original methods if the polynomial degree grows with an order \$\Omega(\log k)\$ at the \$k\$-th iteration. If the warm-start property is considered, the degree can be reduced to a constant, independent of the iteration \$k\$. Preliminary numerical experiments on several low-rank matrix optimization problems show that the polynomial filtered algorithms usually provide multi-fold speedups.

#### PDE-Net 2.0: Learning PDEs from Data with A Numeric-Symbolic Hybrid Deep Network

#### 龙子超

#### 北京大学 zlong@pku.edu.cn

Partial differential equations (PDEs) are commonly derived based on empirical observations. However, recent advances of technology enable us to collect and store massive amount of data, which offers new opportunities for data-driven discovery of PDEs. In this paper, we propose a new deep neural network, called PDE-Net 2.0, to discover (time-dependent) PDEs from observed dynamic data with minor prior knowledge on the underlying mechanism that drives the dynamics. The design of PDE-Net 2.0 is based on our earlier work \cite{Long2018PDE} where the original version of PDE-Net was proposed. PDE-Net 2.0 is a combination of numerical approximation of differential operators by convolutions and a symbolic multi-layer neural network for model recovery. Comparing with existing approaches, PDE-Net 2.0 has the most flexibility and expressive power by learning both differential operators and the nonlinear response function of the underlying PDE model. Numerical experiments show that the PDE-Net 2.0 has the potential to uncover the hidden PDE of the observed dynamics, and predict the dynamical behavior for a relatively long time, even in a noisy environment.

#### 2D EVP, Newton method, and RQI method 陆天怡 复旦大学 17110840004@fudan.edu.cn

The 2D eigenvalue problem (2D EVP) is a class of the 2-parameter eigenvalue problems first studied by Blum and Chang in 1970s. The 2D EVP seeks real scalars

#### SAV schemes for the binary fluid-surfactant system 秦煜哲 北京师范大学 yzqin@mail.bnu.edu.cn

Here, we develop a first and a second order time stepping schemes for a binary fluid-surfactant phase field model by using the scalar auxiliary variable approach. The free energy contains a double-well potential, a nonlinear coupling entropy and a Flory-Huggins potential. The resulting coupled system consists of a Cahn-Hilliard type equation and a Wasserstein type equation which leads to a degenerate problem. By introducing one scalar auxiliary variable, the system is transformed into an equivalent form so that the nonlinear terms can be treated semi-explicitly. Both the schemes are linear and decoupled, thus they can be solved efficiently. We further prove that these semi-discretized schemes in time are unconditionally energy stable. Some numerical experiments are performed to validate the accuracy and energy stability of the proposed schemes.

## 二十面体准晶的稳定性研究以及相场模型时间自适应策略

司伟

#### 湘潭大学 18156921965@163.com

我们采用投影方法,基于多序参量的 Swift-Hohenberg 模型对二十面体准晶的稳 定性进行了研究.通过对多种有序结构的自由能比较,结果显示二十面体准晶可以在相 图中稳定存在.为了加快动力学方程的收敛速度,我们提出了时间自适应的加速近似梯 度法.对离散的能量泛函,该方法可以证明是保证能量耗散和收敛的.

#### The relationship between PDE and deep neural networks 陶文启

#### 清华大学 twq17@mails.tsinghua.edu.cn

In this talk, I will discuss the relationship between PDE and deep neural

networks. A new network modeled by using numerical methods of PDE will be introduced.The new network can improve testing accuracy and robustness towards adversarial attack.

## 3D \$H^2\$-nonconforming tetrahedral finite elements for the biharmonic equation

#### 田舒丹

#### 北京大学 tianshudan@pku.edu.cn

We introduce a family of \$H^2\$-nonconforming finite elements on tetrahedral grids for solving the biharmonic equation in 3D.

In the family, the \$P\_\ell\$ polynomial space is enriched by some high order polynomials for all \$\ell\ge 3\$ and the corresponding finite element solution converges at the optimal order \$\ell-1\$ in \$H^2\$ norm. Moreover, the result is improved for two low order cases by using \$P\_6\$ and \$P\_7\$ polynomials to enrich \$P\_4\$ and \$P\_5\$ polynomial spaces, respectively. The optimal order error estimate is proved.

#### Inclination angle between dislocations and free surface 王封儒 武汉大学 wangfr@whu.edu.cn

We have developed a continuous model to describe the inclination of a dislocations near a free surface in BCC crystal. In this model, an energy variation equation is set to obtain the force balance between the effect of energy difference in different lattice orientation and the influence of the free surface. As a result, the relationship between the inclination angle of the dislocations and the tilt of the Burgers vector is given. We have also numerically simulated our model with Molecular Dynamics method, which verifies the validity of our model for the results from coutinuous model matches with the numerical simulation.

#### A Pseudo Moving Mesh Method for Flow Solver Acceleration in Aerodynamic Optimization

#### 王居方

北京航空航天大学 wangjufang@buaa.edu.cn

Generally, in the aerodynamic optimization problem based on computational fluid dynamics (CFD), the aerodynamic shape is represented and deformed by the

design variables based on specific geometry parameterization method, and the objective to be optimized is considered as a function of the design variables. Once the design variables are updated, a new shape is obtained, and the objective of the new shape is evaluated by CFD simulation including mesh generation or deformation and flow computation with numerical solvers. Therefore, a large number of objective function evaluations are required for an optimal design, and an efficient flow computation for the function evaluation becomes crucial to reduce the time cost of the entire optimization process.

In this talk, a pseudo moving mesh method is presented and applied to the transonic airfoil design problem to provide a fast convergence of solving the compressible Euler equations for the given flow solver; once the flow solution for the current airfoil shape is obtained, the initial value for the next shape is constructed by mimicking the moving mesh strategy, where the mesh of the current shape is assumed to move to the one of the next shape due to the small perturbation of the shape. Based on this strategy, the formula of deploying the initial value for the next shape is derived. Numerical experiments show that the present strategy of initial value deployment can attractively accelerate flow convergence and reduce computational time in the optimization process.

## 复杂多孔介质流体的弱有限元方法 王秀丽

吉林大学 xiuli16@mails.jlu.edu.cn

In this paper, we apply the weak Galerkin (WG) finite element method to the Darcy-Stokes equation. In the WG method, the finite element spaces are made up of piecewise polynomials without continuous constraints. The WG method can be applied to the polygonal meshes and the finite element space is easy to construct, which makes the WG method highly flexible and efficient. Optimal convergence rates independent of viscosity of the flow e for uh and ph in corresponding norms are established. Several numerical experiments are provided to illustrate the theoretical analysis.

> Recent Progress on Multiscale Coupling Methods 王阳帅 上海交大 yswang2016@sjtu.edu.cn

Some In this talk I will briefly introduce several recent progress on multiscale coupling methods. Nonlinear elastic models are widely used to describe the elastic response of crystalline solids, for example, the well-known Cauchy-Born model. While the Cauchy-Born model only depends on the strain, effects of higher order strain gradients are significant and higher order continuum models are preferred, in various applications such as defect dynamics and modeling of carbon nanotubes. We rigorously derive a higher order nonlinear elasticity model for crystals from its atomistic description in one dimension. We show that, compared to the second order accuracy of the Cauchy-Born model, the higher order continuum model in this paper is of fourth order accuracy. QM (quantum mechanics) and MM (molecular mechanics) coupling methods are widely used in simulations of crystalline defects. We construct a residual based a posteriori error indicator for QM/MM coupling approximations. We prove the reliability of the error indicator and design an adaptive QM/MM algorithm for crystalline defects and demonstrate the efficiency with some numerical experiments. We also propose an efficient multigrid strategy for large-scale molecular mechanics optimization. The coarse-grid problem is constructed from the atomistic model systematically on-the-fly using a quasi-atomistic approximation. The oneway multigrid method is used with inexact approximations at coarse levels which are adaptively generated. The numerical experiments show the efficiency of the strategy. These are the joint works with Prof. Christoph Ortner (UW), Prof. Lei Zhang (SJTU), Prof. Huajie Chen (BNU) and Prof. Hao Wang (SCU).

#### A novel alternating-direction implicit spectral Galerkin method for a multiterm time-space fractional diffusion equation in three dimensions 王莹

西安交通大学 wangying920409@163.com

In this paper, we develop an efficient spectral Galerkin method for the threedimensional multi-term time-space fractional diffusion equation. Based on \$L2\$-\$1\sigma\$ formula for time stepping and the Legendre-Galerkin spectral method for space discretization, a fully discrete numerical scheme is constructed and the stability and convergence analysis are rigorously established. The results show that the fully discrete scheme is unconditionally stable and has second-order accuracy in time and optimal error estimation in space. In addition, we give the detailed implementation and apply the alternating-direction implicit method to reduce the computational complexity. Furthermore, numerical experiments are presented to confirm the theoretical claims. As the applications of the proposed method, the fractional Bloch-Torrey model is also solved.

### Coordinate-wise Descent Methods for the Full Configuration Interaction Calculation

#### 王喆

#### 杜克大学 zhe.wang3@duke.edu

The full configuration interaction (FCI) calculation computes the smallest eigenvalue of a sparse symmetric matrix. While the computational challenge of the FCI calculation lies in the fact that the matrix size grows exponentially with respect to the number of orbitals/electrons in the system. In this work, the coordinate-wise descent methods are considered for such problems based on a reformulation of the edge eigenvalue problem as a non-convex optimization problem. Numerical examples of physical systems demonstrate the efficiency and provide benchmarks of the FCI calculation.

#### 

北京大学 xiongyf1990@pku.edu.cn

Towards to an efficient stochastic simulations of the Wigner quantum dynamics in high dimensional (\$\geq\$6D) phase space, the variance reduction plays a key role, which can be achieved by a weighted-particle implementation with the fractional particle weights adopted. Unfortunately, such manner may lead to a large growth rate of particle number and consequently increases the computational complexity. Under the mathematical framework of branching random walk solutions to the Wigner equation, we introduce a new way to control the variance and computational complexity simultaneously, thereby essentially improving the efficiency of the existing stochastic algorithms. Theoretical analysis validates the accuracy of the proposed method and numerical results also demonstrate its reliability.

a sequential least squares method for elliptic problem in non-divergence

#### form

#### 杨凡意

#### 北京大学 yangfanyi@pku.edu.cn

We develop a new least squares method for solving the second-order elliptic equations in non-divergence form. Two least-squares-type functionals are proposed for solving the equations in two steps. We first obtain a numerical approximation to the gradient in a piecewisely irrotational polynomial space. Then together with the numerical gradient, we seek a numerical solution of the primitive variable in continuous finite element space. The error estimates in L<sup>2</sup> norm and energy norms for both two unknowns are derived. By a series of numerical experiments, we verify the convergence rates.

### Solving Heated Oil Pipeline Problems Via Mixed Integer Nonlinear Programming Approach

杨沐明

中国科学院 ymm@lsec.cc.ac.cn

It is a crucial problem how to heat oil and save running cost for crude oil transport. This work strictly formulates such a heated oil pipeline problem as a mixed integer nonlinear programming model. Nonconvex and convex continuous relaxations of the model are proposed, which are proved to be equivalent under some suitable conditions. Meanwhile, we provide a preprocessing procedure to guarantee these conditions. Therefore we are able to design a branch-and-bound algorithm for solving the mixed integer nonlinear programming model to global optimality. To make the branch-and-bound algorithm more efficient, an outer approximation method is proposed as well as the technique of warm start is used. The numerical experiments with a real heated oil pipeline problem show that our algorithm achieves a better scheme and can save 6.83% running cost compared with the practical scheme.

#### Construct solution landscapes of nematic liquid crystals 殷鉴远 北京大学 yinjy@pku.edu.cn

In this talk, we present a solution landscape as an extension of the energy landscape. The solution landscape is a directed graph consisting of all stationary points of an energy functional and their connections. Based on the high-index optimization-based shrinking dimer method, we develop a numerical algorithm for constructing the solution landscape efficiently. As an application, we construct the solution landscapes of nematic liquid crystals confined in a square well, which are described by the modified Oseen-Frank model or the Landau-de Gennes model. Two stable configuarations known as diagonal and rotated solutions appear in both models. For different domain sizes, various states can be systematically discovered and well-explained using solution landscapes. Furthermore, the solution landscapes can help us comprehend the similarities and differences between two models when defects exists.

## The Kohn-Sham density functional theory model: From the optimization point of view

张力维 中国科学院 zhanglw@lsec.cc.ac.cn

This talk includes some of our recent works on solving the Kohn-Sham DFT model from the optimization point of view. In the first part of the talk, we introduce the conjugate gradient method for electronic structure calculations. We have proved its convergence and successfully applied the algorithm to some typical systems (including large systems up to thousands of atoms). In the second part of the talk, we propose an adaptive step size strategy for a class of line search methods with orthogonality constraints which avoids the classic backtracking procedure and outperforms the classic step size strategy.

#### A simple iterative algorithm for maxcut 张维熹 北京大学 zhangweixi@pku.edu.cn

We propose a simple iterative (SI) algorithm for the maxcut problem through fully using an equivalent continuous formulation. It has advantages that all subproblems have explicit analytic solutions, the cut value is monotonic updated and its iteration points converge to a local optima in finite steps via an appropriate subgradient selection.

A hybrid Hermite WENO scheme for hyperbolic conservation laws 赵状 厦门大学 zzhao@stu.xmu.edu.cn

In this presentation, we propose a hybrid finite volume Hermite weighted essentially non-oscillatory (HWENO) scheme for solving one and two dimensional hyperbolic conservation laws. The zeroth-order and the first-order moments are used in the spatial reconstruction, with total variation diminishing Runge-Kutta time discretization. The main idea of the hybrid HWENO scheme is that we first use a shock-detection technique to identify the troubled cell, then, if the cell is identified as a troubled cell, we would modify the first order moment in the troubled cell and employ HWENO reconstruction in spatial discretization; otherwise, we directly use high order linear reconstruction. Unlike other HWENO schemes, we borrow the thought of limiter for discontinuous Galerkin (DG) method to control the spurious oscillations, after this procedure, the scheme would avoid the oscillations by using HWENO reconstruction nearby discontinuities and have higher efficiency for using linear approximation straightforwardly in the smooth regions. In addition, the hybrid HWENO scheme still keeps the compactness. A collection of benchmark numerical tests for one and two dimensional cases are performed to demonstrate the numerical accuracy, high resolution and robustness of the proposed scheme.

#### Hybridized Discontinuous Galerkin Methods for Helmholtz Equation with High Wave Number

朱冰心

南京大学 867621163@qq.com

This paper presents a Hybridized Discontinuous Galerkin finite element method(HDG) for Helmholtz equation with the first order absorbing boundary condition in one, two and three dimensions. We drive the  $H^1-$  and  $L^2-$  error estimates with explicit dependence on the wave number k. It is shown that if  $k^3h^2$  is sufficiently small, then the pollution errors of HDG method in  $H^1$ -norm are bounded by O( $k^4h^3$ ), which coincides with the phase error of the finite element method obtained by existent dispersion analysis on Cartesian grids, where h is the mesh size. In general, we can get that if  $k(k)^{p+1}$  is sufficiently small, then the pollution errors of HDG method in  $H^1$ -norm are bounded by  $O(k(kh)^{2p+1})$ , where p is the fixed order of the approximation space. Some numerical experiments are provided to verify our theoretical results and to illustrate great capability of the symmetric HDG method

in reducing the pollution error effect.