

第十一届全国计算数学年会

2017年7月21-23日

中国 西安

主办单位: 中国数学会计算数学分会

承办单位: 西北工业大学 中国科学院计算数学与科学工程计算研究所

资助单位: 国家自然科学基金委员会

会议委员会

一、会议学术委员会

主席:

鄂维南 院士 (北京大学, 中国数学会计算数学分会理事长)

汪劲松 教授 (西北工业大学, 校长)

委员 (按姓氏拼音排序):

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崔俊芝 院士 (中国科学院)

江 松 院士 (北京应用物理与计算数学研究所, 中国数学会计算数学分会副理事长)

林 群 院士 (中国科学院)

石钟慈 院士 (中国科学院, 中国数学会计算数学分会名誉理事长)

舒其望 教授 (美国布朗大学, 中国科技大学, 中国数学会计算数学分会指导委员会主任)

宋永忠 教授 (南京师范大学, 中国数学会计算数学分会副理事长)

许跃生 教授 (中山大学, 中国数学会计算数学分会副理事长)

羊丹平 教授 (华东师范大学, 中国数学会计算数学分会副理事长)

袁亚湘 院士 (中国科学院, 中国数学会理事长, 中国数学会计算数学分会指导委员会主任)

张平文 院士 (北京大学, 中国工业与应用数学学会理事长)

二、会议组织委员会

主席:

宋永忠 教授 (南京师范大学, 中国数学会计算数学分会副理事长)

许志强 研究员 (中国科学院, 中国数学会计算数学分会秘书长)

聂玉峰 教授 (西北工业大学, 理学院副院长)

委员 (按姓氏拼音排序):

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凤小兵 教授 (美国田纳西大学, 西北工业大学)

蔡 力 副教授 (西北工业大学, 应用数学系副主任)

分项联系人:

注册: 余红伟 (13227792078)、王晓东 (13389245201)

学术: 王俊刚 (15091770883)、袁占斌 (18309215152)

住宿: 王振海 (13193301470)、杨自豪 (15398004619)、赵丽静 (15721918826)

会场: 张伟伟 (13759912419)、王淑琴 (15991698368)、马 啸 (18729061185)

交通: 赵俊锋 (18049405436)、肖曼玉 (15229313508)

餐饮: 王晓龙 (13679275419)、延伟东 (15319730745)

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一 会场信息及简要日程

会议场地信息

开幕式与所有的大会报告均在陕西宾馆大礼堂。分会场信息详见下表。

会场位置	会场名称
10 号楼 6 层	第一会议室
10 号楼 6 层	第二会议室
12 号楼 2 层	第一会议室
12 号楼 3 层	第三会议室
19 号楼 2 层	第二会议室
19 号楼 2 层	第三会议室
19 号楼 2 层	第四会议室
19 号楼 2 层	第五会议室
19 号楼 2 层	第九会议室
19 号楼 2 层	第十会议室

注: 19 号楼即为西安陕宾馆国际酒店。

简要日程

时间	7 月 21 日	7 月 22 日	7 月 23 日
08:30–10:00	开幕式 8:30-8:45	徐宗本院士 8:30-9:15	杨超研究员 8:30-9:15
	颁奖典礼 8:45-9:40		张然教授 9:15-10:00
	学会工作报告 9:40-10:00	陈龙教授 9:15-10:00	
10:00–10:30	茶歇	茶歇	茶歇
10:30–12:00	李若教授 10:30-11:15	凤小兵教授 10:30-11:15	张志华教授 10:30-11:15
	吴国宝教授 11:15-12:00	韩德仁教授 11:15-12:00	郑伟英研究员 11:15-12:00
12:00–13:30	午餐	午餐	午餐
14:00–16:00	分会场报告 1 S02-1 S06-1 S07-1 S08-1 S11-1 S13-1 T01-1 T03-1 T06-1 T09-1	分会场报告 3 S01-1 S03-1 S04-1 S05-1 S09-1 T01-3 T06-3 T07-1 T09-3	分会场报告 5 S10-1 S12-1 T02-1 T04-1 T06-5 T08-1 T10-1 T11-1 T12-1
16:00–16:20	茶歇	茶歇	茶歇
16:20–18:00	分会场报告 2 S06-2 S07-2 S08-2 S11-2 S13-2 T01-2 T03-2 T05-1 T06-2 T09-2	分会场报告 4 S01-2 S03-2 S04-2 S05-2 S08-3 T02-3 T05-2 T06-4 T09-4	分会场报告 6 S01-3 S10-2 S12-2 T02-2 T04-2 T08-2 T09-5 T12-2
18:30–20:00	晚餐	晚餐	晚餐

注 1: 常务理事会于 7 月 20 日 19:00 在 19 号楼第三会议室举行。

注 2: 计算数学青年优秀论文奖评选于 7 月 21 日 19:30 在 19 号楼第三会议室举行。

注 3: 分会场主持人和组织者可以在不影响茶歇时间的前提下根据报告数目酌情调整报告时间。

粗略主题分类及其编号

T01	微分方程数值计算及应用
T02	流体力学中的数值计算
T03	优化、控制及反问题
T04	数值代数
T05	谱方法、数值逼近与计算几何
T06	有限元和边界元方法
T07	多重网格技术、区域分解及并行计算
T08	自适应方法
T09	分数阶方程
T10	随机微分方程
T11	有限差分法及其应用
T12	移动网格和无网格及有限体积法

专题讨论会及其编号

S01	PDE 并行、快速算法研究进展
S02	非线性色散方程的数值方法
S03	界面问题的建模与计算
S04	材料科学的可计算建模与计算方法
S05	Recent advances in nonstandard discretization methods in scientific and engineering computation
S06	偏微分方程反问题及其计算
S07	流体力学方程的数学理论和数值方法
S08	无界域数学物理方程的数值方法及其应用
S09	Krylov 子空间算法及预处理技术
S10	有限体积法理论及其应用
S11	最优化专题
S12	稀有事件及其鞍点问题的计算与应用
S13	生命科学中的计算数学

二 主会场日程

7月21日上午大会日程

08:30–08:45	开幕式 校领导及嘉宾致辞 主持人：许志强
08:45–09:40	颁奖典礼 青年创新奖颁奖典礼 颁奖嘉宾：江松 获奖人：徐岩, 许志强, 杨周旺 冯康奖颁奖典礼 颁奖嘉宾：鄂维南, 崔俊芝 获奖人：李若, 吴国宝 获奖人工作介绍：张平文, 汤涛
09:40–10:00	学会工作报告 报告人：理事长 鄂维南
10:00–10:30	茶歇
10:30–11:15	冯康科学计算奖获得者报告 报告人：李若 教授 (北京大学) 题目： 动力学方程的模型约化 主持人：陈志明
11:15–12:00	冯康科学计算奖获得者报告 报告人：吴国宝 教授 (香港浸会大学) 题目： Multiple Relational Ranking in Tensor: Theory, Algorithms and Applications 主持人：袁亚湘

7月22日上午大会日程

08:30–09:15	报告人: 徐宗本 院士 (西安交通大学) 题目: 大数据分析技术图谱与研究举例 主持人: 聂玉峰
09:15–10:00	报告人: 陈龙 教授 (University of California at Irvine) 题目: Mixed Finite Element Methods based on Differential Complexes 主持人: 聂玉峰
10:00–10:30	茶歇
10:30–11:15	报告人: 凤小兵 教授 (美国田纳西大学, 西北工业大学) 题目: Fully Nonlinear Second Order PDEs and Their Numerical Solutions 主持人: 宋永忠
10:30–11:15	报告人: 韩德仁 教授 (南京师范大学) 题目: Alternating direction methods with multipliers for optimization problems involving nonconvex functions 主持人: 宋永忠

7月23日上午大会日程

08:30–09:15	报告人: 杨超 研究员 (中国科学院软件研究所) 题目: 千万核可扩展全隐式求解器: 算法、实现与应用 主持人: 包刚
09:15–10:00	报告人: 张然 教授 (吉林大学) 题目: Weak Galerkin Finite Element Scheme and Its Applications 主持人: 包刚
10:00–10:30	茶歇
10:30–11:15	报告人: 张志华 教授 (北京大学) 题目: 大规模矩阵近似的随机算法 主持人: 羊丹平
11:15–12:00	报告人: 郑伟英 研究员 (中国科学院数学与系统科学研究院) 题目: 三维不可压磁流体方程组的并行计算方法 主持人: 羊丹平

三 分会场和专题报告日程简表

分会场报告 1 | 7 月 21 日 14:00-16:00

S02-1 非线性色散方程的数值方法

19 号楼 2 层, 第三会议室

组织者:	蔡勇勇, 王汉权			
报告人:	王汉权	王燕	易雯帆	蔡勇勇
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	王廷春	蒋维		
时间:	15:20-15:40	15:40-16:00		

S06-1 偏微分方程反问题及其计算

19 号楼 2 层, 第四会议室

组织者:	刘晓东			
报告人:	郭玉坤	陆帅	杨家青	曲凤龙
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	王海兵			
时间:	15:20-15:40			

S07-1 流体力学方程的数学理论和数值方法

19 号楼 2 层, 第十会议室

组织者:	汤华中, 成娟			
报告人:	黄飞敏	刘铁钢	邱建贤	汤华中
时间:	14:00-14:30	14:30-15:00	15:00-15:30	15:30-16:00

S08-1 无界域数学物理方程的数值方法及其应用

19 号楼 2 层, 第九会议室

组织者:	武海军, 张继伟, 郑春雄			
报告人:	杨志坚	陈黄鑫	崔涛	胡光辉
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	张继伟			
时间:	15:20-15:40			

S11-1 最优化专题

12 号楼 2 层, 第一会议室

组织者:	戴戡虹, 杨庆之			
报告人:	何炳生	戴戡虹	倪谷炎	宋义生
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	陶敏			
时间:	15:20-15:40			

S13-1 生命科学中的计算数学

19 号楼 2 层, 第五会议室

组织者:	李铁军, 周栋焯			
报告人:	刘娟	卢本卓	牛原玲	王奇
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	吴昊			
时间:	15:20-15:40			

T01-1 微分方程数值计算及应用

10 号楼 6 层, 第一会议室

主持人:	乔中华, 李崇君, 叶颀			
报告人:	李崇君	叶颀	乔中华	王廷春
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	杨旭光	贾亚男		
时间:	15:20-15:35	15:35-15:50		

T03-1 优化、控制及反问题

19 号楼 2 层, 第二会议室

主持人:	祝志川, 文有为, 贾志刚			
报告人:	文有为	贾志刚	祝志川	武婷婷
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:15
报告人:	张理评	崔宰珪		
时间:	15:15-15:30	15:30-15:45		

T06-1 有限元和边界元方法

12 号楼 3 层, 第三会议室

主持人:	易年余, 肖源明, 司智勇			
报告人:	肖源明	司智勇	易年余	杨艳
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:15
报告人:	胡嘉顺	WU Chengda	秦芳芳	
时间:	15:15-15:30	15:30-15:45	15:45-16:00	

T09-1 分数阶方程

10 号楼 6 层, 第二会议室

主持人:	廖洪林, 李常品, 孙志忠			
报告人:	李常品	孙志忠	廖洪林	孙涛
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	李晓	韦雷雷		
时间:	15:20-15:35	15:35-15:50		

分会场报告 2 | 7 月 21 日 16:20-18:00

S06-2 偏微分方程反问题及其计算

19 号楼 2 层, 第四会议室

组织者:	刘晓东			
报告人:	徐翔	张磊 (HLJU)	张海文	
时间:	16:20-16:40	16:40-17:00	17:00-17:20	

S07-2 流体力学方程的数学理论和数值方法

19 号楼 2 层, 第十会议室

组织者:	汤华中, 成娟			
报告人:	蔡力	陈艺冰	李刚	袁海专
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40
报告人:	钟杏慧			
时间:	17:40-18:00			

S08-2 无界域数学物理方程的数值方法及其应用

19 号楼 2 层, 第九会议室

组织者:	武海军, 张继伟, 郑春雄			
报告人:	赖俊	李步扬	陆雅言	邵嗣烘
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40

S11-2 最优化专题

12 号楼 2 层, 第一会议室

组织者:	戴戡虹, 杨庆之			
报告人:	蔡邢菊	白敏茹	魏益民	
时间:	16:20-16:40	16:40-17:00	17:00-17:20	

S13-2 生命科学中的计算数学

19 号楼 2 层, 第五会议室

组织者:	李铁军, 周栋焯			
报告人:	张磊	李铁军	周栋焯	
时间:	16:20-16:40	16:40-17:00	17:00-17:20	

T01-2 微分方程数值计算及应用

10 号楼 6 层, 第一会议室

主持人:	刘雪娇, 王涵, 倪冉			
报告人:	王涵	倪冉	刘雪娇	
时间:	16:20-16:40	16:40-16:55	16:55-17:10	

T03-2 优化、控制及反问题

19 号楼 2 层, 第二会议室

主持人:	张永金, 徐英祥, 郭双冰			
报告人:	徐英祥	郭双冰	张永金	
时间:	16:20-16:40	16:40-16:55	16:55-17:10	

T05-1 谱方法、数值逼近与计算几何

19 号楼 2 层, 第三会议室

主持人:	李金, 王同科, 吴善和			
报告人:	王同科	吴善和	李金	王敏
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:35
报告人:	翟佳音			
时间:	17:35-17:50			

T06-2 有限元和边界元方法

12 号楼 3 层, 第三会议室

主持人:	冯春生, 董巧丽, 夏银华			
报告人:	董巧丽	夏银华	冯春生	张进
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:35
报告人:	张百驹			
时间:	17:35-17:50			

T09-2 分数阶方程

10 号楼 6 层, 第二会议室

主持人:	杨雪花, 蔡好涛, 任金城			
报告人:	蔡好涛	任金城	杨雪花	张海湘
时间:	16:20-16:40	16:40-17:00	17:00-17:15	17:15-17:30
报告人:	黄朝宝	郝朝鹏		
时间:	17:30-17:45	17:45-18:00		

分会场报告 3 | 7 月 22 日 14:00-16:00

S01-1 PDE 并行、快速算法研究进展

12 号楼 2 层, 第一会议室

组织者:	蔡小川, 黄记祖, 陈荣亮			
报告人:	刘杰	张玉	徐小文	杨自豪
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	盛志强			
时间:	15:20-15:40			

S03-1 界面问题的建模与计算

19 号楼 2 层, 第四会议室

组织者:	邸亚娜, 于海军, 许现民			
报告人:	张辉	徐岩	杨将	郑伟英
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	蔡勇勇	季霞		
时间:	15:20-15:40	15:40-16:00		

S04-1 材料科学的可计算建模与计算方法

19 号楼 2 层, 第三会议室

组织者:	高兴誉, 王涵			
报告人:	陈景润	刘芳	张鉴	邵嗣烘
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	王皓	胡光辉		
时间:	15:20-15:40	15:40-16:00		

S05-1 Recent advances in nonstandard discretization methods in scientific and engineering computation

19 号楼 2 层, 第十会议室

组织者:	胡俊, 谢小平, 徐立伟, 张然			
报告人:	崔金涛	黄建国	黄学海	汪艳秋
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	王坤	吴永科		
时间:	15:20-15:40	15:40-16:00		

S09-1 Krylov 子空间算法及预处理技术

19 号楼 2 层, 第二会议室

组织者:	顾先明			
报告人:	殷俊峰	吴钢	李铁香	牛强
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	张建华	顾先明		
时间:	15:20-15:40	15:40-16:00		

T01-3 微分方程数值计算及应用

10 号楼 6 层, 第一会议室

主持人:	余翌帆, 崔霞, 常静雅			
报告人:	崔霞	常静雅	余翌帆	马召灿
时间:	14:00-14:20	14:20-14:40	14:40-14:55	14:55-15:10
报告人:	朱湘疆			
时间:	15:10-15:25			

T06-3 有限元和边界元方法

12 号楼 3 层, 第三会议室

主持人:	宋伦继, 沈晓芹, 黄佩奇			
报告人:	沈晓芹	黄佩奇	宋伦继	赵纪坤
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:15
报告人:	王疆兴	许竞劫		
时间:	15:15-15:30	15:30-15:45		

T07-1 多重网格技术、区域分解及并行计算

19 号楼 2 层, 第九会议室

主持人:	岳孝强, 姚彦忠, 刘会坡			
报告人:	姚彦忠	刘会坡	岳孝强	袁龙
时间:	14:00-14:25	14:25-14:45	14:45-15:00	15:00-15:15
报告人:	徐飞	黄健	董丽秀	
时间:	15:15-15:30	15:30-15:45	15:45-16:00	

T09-3 分数阶方程

10 号楼 6 层, 第二会议室

主持人:	李步扬, 曹婉容, 阮周生			
报告人:	曹婉容	阮周生	李步扬	赵旭鹰
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:15
报告人:	周知	王冬岭		
时间:	15:15-15:30	15:30-15:50		

分会场报告 4 | 7 月 22 日 16:20-18:00

S01-2 PDE 并行、快速算法研究进展

12 号楼 2 层, 第一会议室

组织者:	蔡小川, 黄记祖, 陈荣亮			
报告人:	罗力	王锋	闫争争	李世顺
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40

S03-2 界面问题的建模与计算

19 号楼 2 层, 第四会议室

组织者:	邸亚娜, 于海军, 许现民			
报告人:	应文俊	蒋维	王何宇	许现民
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40

S04-2 材料科学的可计算建模与计算方法

19 号楼 2 层, 第三会议室

组织者:	高兴誉, 王涵			
报告人:	阳莺	李胜国	潘妍	张力维
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40
报告人:	高兴誉			
时间:	17:40-18:00			

S05-2 Recent advances in nonstandard discretization methods in scientific and engineering computation

19 号楼 2 层, 第十会议室

组织者:	胡俊, 谢小平, 徐立伟, 张然			
报告人:	谢和虎	谢小平	张然	张世全
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40
报告人:	张硕			
时间:	17:40-18:00			

S08-3 无界域数学物理方程的数值方法及其应用

19 号楼 2 层, 第九会议室

组织者:	武海军, 张继伟, 郑春雄			
报告人:	武海军	徐立伟	应文俊	张磊
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40
报告人:	郑伟英			
时间:	17:40-18:00			

T02-3 流体力学中的数值计算

10 号楼 6 层, 第一会议室

主持人:	王晓东, 曾清红, 沈智军			
报告人:	曾清红	沈智军	王晓东	龚跃政
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:35
报告人:	孔慧慧			
时间:	17:35-17:50			

T05-2 谱方法、数值逼近与计算几何

19 号楼 2 层, 第二会议室

主持人:	刘飞, 安静, 李昭祥			
报告人:	安静	李昭祥	刘飞	廖锋
时间:	16:20-16:40	16:40-17:00	17:00-17:15	17:15-17:30
报告人:	刘伟	高天成		
时间:	17:30-17:45	17:45-18:00		

T06-4 有限元和边界元方法

12 号楼 3 层, 第三会议室

主持人:	魏华祎, 姚昌辉, 黄红英			
报告人:	姚昌辉	黄红英	魏华祎	王梦莹
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:35
报告人:	马利敏			
时间:	17:35-17:50			

T09-4 分数阶方程

10 号楼 6 层, 第二会议室

主持人:	孟祥云, 闫玉斌, 祁瑞生			
报告人:	闫玉斌	祁瑞生	孟祥云	张治江
时间:	16:20-16:40	16:40-16:55	16:55-17:10	17:10-17:25
报告人:	李猛	纪翠翠		
时间:	17:25-17:40	17:40-17:55		

分会场报告 5 | 7 月 23 日 14:00-16:00

S10-1 有限体积法理论及其应用

12 号楼 2 层, 第一会议室

组织者:	邹青松, 李永海			
报告人:	林延平	邹青松	王翔	邬吉明
时间:	14:00-14:20	14:20-14:40	14:40-14:55	14:55-15:15
报告人:	张志跃			
时间:	15:15-15:35			

S12-1 稀有事件及其鞍点问题的计算与应用

19 号楼 2 层, 第二会议室

组织者:	张磊, 任维清, 杨志坚			
报告人:	周翔	李铁军	汪涵	于海军
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	Ran NI			
时间:	15:20-15:40			

T02-1 流体力学中的数值计算

19 号楼 2 层, 第十会议室

主持人:	徐骁, 黄鹏展, 许晓阳			
报告人:	黄鹏展	许晓阳	徐骁	陈锐
时间:	14:00-14:20	14:20-14:40	14:40-14:55	14:55-15:10
报告人:	曹雅茹	王华	赵立飞	
时间:	15:10-15:30	15:30-15:45	15:45-16:00	

T04-1 数值代数

10 号楼 6 层, 第一会议室

主持人:	吴庆标, 白正简, 高卫国			
报告人:	白正简	高卫国	吴庆标	卢欣
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:15
报告人:	郭培昌	张瑞	王会迪	
时间:	15:15-15:30	15:30-15:45	15:45-16:00	

T06-5 有限元和边界元方法

10 号楼 6 层, 第二会议室

主持人:	王淑琴, 王飞, 葛志昊			
报告人:	王飞	葛志昊	王淑琴	王海金
时间:	14:00-14:20	14:20-14:40	14:40-14:55	14:55-15:10

T08-1 自适应方法

12 号楼 3 层, 第三会议室

主持人:	吕俊良, 朱洪强, 龚伟			
报告人:	朱洪强	龚伟	吕俊良	刘利斌
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:15
报告人:	王利娜			
时间:	15:15-15:30			

T10-1 随机微分方程

19 号楼 2 层, 第四会议室

主持人:	郭谦, 徐承龙, 姜立建			
报告人:	徐承龙	姜立建	郭谦	袁海燕
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:20
报告人:	付余	逯伯亮	刘永乐	
时间:	15:20-15:35	15:35-15:50	15:50-16:05	

T11-1 有限差分法及其应用

19 号楼 2 层, 第三会议室

主持人:	高理平, 杭旭登, 冯秀芳			
报告人:	杭旭登	冯秀芳	高理平	钱旭
时间:	14:00-14:20	14:20-14:40	14:40-15:00	15:00-15:15
报告人:	王姗姗	周旋旋	鲜双燕	
时间:	15:15-15:30	15:30-15:45	15:45-16:00	

T12-1 移动网格和无网格及有限体积法

19 号楼 2 层, 第九会议室

主持人:	彭洁, 李小林, 冯仁忠			
报告人:	李小林	冯仁忠	彭洁	张齐
时间:	14:00-14:20	14:20-14:40	14:40-14:55	14:55-15:10

分会场报告 6 | 7 月 23 日 16:20-18:00

S01-3 PDE 并行、快速算法研究进展

19 号楼 2 层, 第三会议室

组织者:	蔡小川, 黄记祖, 陈荣亮			
报告人:	蔡小川	黄记祖	徐磊	
时间:	16:20-16:40	16:40-17:00	17:00-17:20	

S10-2 有限体积法理论及其应用

12 号楼 2 层, 第一会议室

组织者:	邹青松, 李永海			
报告人:	何文明	曹外香	刘玉洁	张庆辉
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40
报告人:	高志明			
时间:	17:40-18:00			

S12-2 稀有事件及其鞍点问题的计算与应用

19 号楼 2 层, 第二会议室

组织者:	张磊, 任维清, 杨志坚			
报告人:	张亚楠	靳聪明	张磊	
时间:	16:20-16:40	16:40-17:00	17:00-17:20	

T02-2 流体力学中的数值计算

19 号楼 2 层, 第十会议室

主持人:	彭秋瑾, 李义宝, 叶挺			
报告人:	李义宝	叶挺	彭秋瑾	徐真
时间:	16:20-16:40	16:40-17:00	17:00-17:15	17:15-17:30
报告人:	李晓丽	赵刚		
时间:	17:30-17:45	17:45-18:00		

T04-2 数值代数

10 号楼 6 层, 第一会议室

主持人:	杨畅, 吕长青, 杜魁			
报告人:	吕长青	杜魁	杨畅	吴静
时间:	16:20-16:40	16:40-17:00	17:00-17:15	17:15-17:30
报告人:	李凌霄			
时间:	17:30-17:45			

T08-2 自适应方法

12 号楼 3 层, 第三会议室

主持人:	刘剑明, 满红英, 毛士鹏			
报告人:	满红英	毛士鹏	刘剑明	张蓓
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:35

T09-5 分数阶方程

10 号楼 6 层, 第二会议室

主持人:	许传炬, 王宏, 徐大			
报告人:	王宏	徐大	许传炬	陈明华
时间:	16:20-16:40	16:40-17:00	17:00-17:20	17:20-17:40

T12-2 移动网格和无网格及有限体积法

19 号楼 2 层, 第九会议室

主持人:	赵腾进, 鲁祖亮, 杨晓波			
报告人:	鲁祖亮	杨晓波	赵腾进	
时间:	16:20-16:40	16:40-16:55	16:55-17:10	

四 分会场和专题报告详细内容

分会场报告 1

S02-1 非线性色散方程的数值方法

时间: 7 月 21 日 14:00-16:00 会场: 19 号楼 2 层, 第三会议室

组织者: 蔡勇勇(北京计算科学研究中心)

王汉权(云南财经大学)

报告人	题目
王汉权 (14:00-14:20) 云南财经大学	An efficient time-splitting compact finite difference method for nonlinear Schrodinger-type equations
王燕 (14:20-14:40) 北京计算科学研究中心	A uniformly accurate multiscale time integrator pseudospectral method for the nonlinear Dirac equation in the nonrelativistic limit regime
易雯帆 (14:40-15:00) 北京计算科学研究中心	Error bounds of finite difference time domain (FDTD) methods for the Dirac-Klein-Gordon equations
蔡勇勇 (15:00-15:20) 北京计算科学研究中心	Error estimates of finite difference method for Zakharov system in the subsonic limit
王廷春 (15:20-15:40) 南京信息工程大学	Unconditional convergence of an alternating direction implicit finite difference scheme for the nonlinear Schrodinger equation in two dimensions
蒋维 (15:40-16:00) 武汉大学	Mathematical models and simulations for solid-state dewetting problems

S06-1 偏微分方程反问题及其计算**时间:** 7月21日 14:00-16:00 **会场:** 19号楼2层, 第四会议室**组织者:** 刘晓东(中国科学院数学与系统科学研究院)

报告人	题目
郭玉坤 (14:00-14:20) 哈尔滨工业大学	Fourier method for the multi-frequency inverse source problems
陆帅 (14:20-14:40) 复旦大学数学科学学院	Increasing stability in the inverse source problem with attenuation and many frequencies
杨家青 (14:40-15:00) 西安交通大学	Imaging of a local rough interface in a two-layered medium with possibly buried obstacles
曲凤龙 (15:00-15:20) 烟台大学	Near-field imaging of an inhomogeneous cavity with the factorization method
王海兵 (15:20-15:40) 东南大学	Solvability of interior transmission problem for the diffusion equation and its applications

S07-1 流体力学方程的数学理论和数值方法**时间:** 7月21日 14:00-16:00 **会场:** 19号楼2层, 第十会议室**组织者:** 汤华中(北京大学数学科学学院)

成娟(北京应用物理与计算数学研究所)

报告人	题目
黄飞敏 (14:00-14:30) 中国科学院数学与系统科学研究院	Compressible Euler equations and related problems
刘铁钢 (14:30-15:00) 北京航空航天大学数学与系统科学学院	Direct Discontinuous Galerkin Method with Interface Correction
邱建贤 (15:00-15:30) 厦门大学数学科学学院	A simple and efficient WENO method for hyperbolic conservation laws
汤华中 (15:30-16:00) 北京大学数学科学学院、湘潭大学 数学与计算科学学院	Globally hyperbolic moment model of arbitrary order for special relativistic Boltzmann equation

S08-1 无界域数学物理方程的数值方法及其应用**时间:** 7月21日 14:00-16:00 **会场:** 19号楼2层, 第九会议室**组织者:** 武海军(南京大学)

张继伟(北京计算科学研究中心)

郑春雄(清华大学)

报告人	题目
杨志坚 (14:00-14:20) 武汉大学数学与统计学院	Effective boundary conditions for MD simulations
陈黄鑫 (14:20-14:40) 厦门大学数学科学学院	HDG methods for the Maxwell equations
崔涛 (14:40-15:00) 中国科学院数学与系统科学研究院	并行波源转移区域分裂算法
胡光辉 (15:00-15:20) 澳门大学数学系	Computational Issues on Kohn-Sham Equation
张继伟 (15:20-15:40) 北京计算科学研究中心	Artificial boundary conditions of nonlocal models on unbounded domains

S11-1 最优化专题**时间:** 7月21日 14:00-16:00 **会场:** 12号楼2层, 第一会议室**组织者:** 戴戡虹(中国科学院数学与系统科学研究院)

杨庆之(中国科学院数学与系统科学研究院)

报告人	题目
何炳生 (14:00-14:20) 南方科技大学/南京大学	三个算子的交替方向类算法 (ADMM) 进展
戴戡虹 (14:20-14:40) 中国科学院数学与系统科学研究院	CMIP 混合整数规划求解器进展
倪谷炎 (14:40-15:00) 国防科技大学	复张量特征值计算
宋义生 (15:00-15:20) 河南师范大学	Structured Tensor and Complementarity Problem
陶敏 (15:20-15:40) 南京大学	On Glowinski's Open Question of Alternating Direction Method of Multipliers

S13-1 生命科学中的计算数学**时间:** 7月21日 14:00-16:00 **会场:** 19号楼2层, 第五会议室**组织者:** 李铁军(北京大学)

周栋焯(上海交通大学)

报告人	题目
刘娟 (14:00-14:20) 武汉大学	基于三层数据融合的药物-疾病关系预测模型
卢本卓 (14:20-14:40) 中国科学院	离子通道模型与有限元模拟
牛原玲 (14:40-15:00) 中南大学	The phenotypic equilibrium of cancer cells: From average-level stability to path-wise convergence
王奇 (15:00-15:20) 北京计算科学研究中心、南卡大学	Systematic development of stable numerical methods for nonequilibrium dissipative systems with applications to life science
吴昊 (15:20-15:40) 柏林自由大学	Multiensemble Markov models of molecular thermodynamics and kinetics

T01-1 微分方程数值计算及应用**时间:** 7 月 21 日 14:00-16:00 **会场:** 10 号楼 6 层, 第一会议室**主持人:** 乔中华(香港理工大学)

李崇君(大连理工大学数学科学学院)

叶颀(华南师范大学)

报告人	题目
李崇君 (14:00-14:20) 大连理工大学数学科学学院	线性微分系统重构的数值算法
叶颀 (14:20-14:40) 华南师范大学	Kernel-based Approximation Methods for Partial Differential Equations: Deterministic or Stochastic Problems?
乔中华 (14:40-15:00) 香港理工大学	Recent development in numerical simulations of molecular beam epitaxial equations
王廷春 (15:00-15:20) 南京信息工程大学	Unconditional and optimal H2-error estimates of two linear and conservative finite difference schemes for the Klein-Gordon-Schrodinger equation in high dimensions
杨旭光 (15:20-15:35) 湖南第一师范学院	A mass conserving lattice Boltzmann scheme for diffuse interface model with different equation of states
贾亚男 (15:35-15:50) 南京师范大学	High-accuracy algorithms for one dimensional singular interface problems

T03-1 优化、控制及反问题**时间:** 7 月 21 日 14:00-16:00 **会场:** 19 号楼 2 层, 第二会议室**主持人:** 祝志川(吉林财经大学)

文有为(湖南师范大学)

贾志刚(数学与统计学院/江苏师范大学)

报告人	题目
文有为 (14:00-14:20) 湖南师范大学	Regularization Parameter Selection for Total Variation Based Image Restoration
贾志刚 (14:20-14:40) 数学与统计学院/江苏师范大学	A new TV-Stokes model for image deblurring and denoising with fast algorithms
祝志川 (14:40-15:00) 吉林财经大学	A globally convergent method for computing fixed point of self-mapping on general nonconvex set
武婷婷 (15:00-15:15) 南京邮电大学	An efficient Peaceman-Rachford splitting method for constrained TGV-shearlet based MRI reconstruction
张理评 (15:15-15:30) 浙江工业大学	Tikhonov Regularization and Randomized GSVD
崔宰珪 (15:30-15:45) 上海交通大学	PET-MRI Joint Reconstruction by Joint Sparsity Based Tight Frame Regularization

T06-1 有限元和边界元方法**时间:** 7月21日 14:00-16:00 **会场:** 12号楼3层, 第三会议室**主持人:** 易年余(湘潭大学)

肖源明(南京大学)

司智勇(河南理工大学)

报告人	题目
肖源明 (14:00-14:20) 南京大学	High-Order Extended Finite Element Methods for Solving Interface Problems
司智勇 (14:20-14:40) 河南理工大学	Unconditional stability and error estimates of modified characteristics Finite Element Methods
易年余 (14:40-15:00) 湘潭大学	Mesh quality and more detailed error estimates of finite element method
杨艳 (15:00-15:15) 西南石油大学	low order conforming mixed finite element methods for elasticity on simplicial grids
胡嘉顺 (15:15-15:30) 清华大学	Fast and stable evaluation of the exact absorbing boundary condition for the semi-discrete linear Schrodinger equation in unbounded domains
WU Chengda (15:30-15:45) City University of Hong Kong	Analysis of Galerkin FEMs for mixed formulation of time-dependent Ginzburg-Landau equations under temporal gauge
秦芳芳 (15:45-16:00) 南京师范大学	A Cartesian grid nonconforming immersed finite element method for planar elasticity interface problems

T09-1 分数阶方程**时间:** 7月21日 14:00-16:00 **会场:** 10号楼6层, 第二会议室**主持人:** 廖洪林(解放军陆军工程大学)

李常品(上海大学)

孙志忠(东南大学)

报告人	题目
李常品 (14:00-14:20) 上海大学	The finite difference method for Caputo-type parabolic equation with fractional Laplacian
孙志忠 (14:20-14:40) 东南大学	分数阶双延迟纳米热传导模型和数值方法
廖洪林 (14:40-15:00) 解放军陆军工程大学	Nonuniform L1 formula and discrete Gronwall inequality for time-fractional reaction-subdiffusion equations
孙涛 (15:00-15:20) 上海立信会计金融学院	Mapped Jacobi Spectral Methods for Singularly Perturbed Problems of Fractional Order
李晓 (15:20-15:35) 北京计算科学研究中心	Energy Stable Numerical Schemes for Some Classical and Nonlocal Phase Field Models
韦雷雷 (15:35-15:50) 河南工业大学	Stability and convergence of a fully-discrete local discontinuous Galerkin method for multi-term time fractional diffusion equations

分会场报告 2**S06-2 偏微分方程反问题及其计算****时间:** 7月21日 16:20-18:00 **会场:** 19号楼2层, 第四会议室**组织者:** 刘晓东(中国科学院数学与系统科学研究院)

报告人	题目
徐翔 (16:20-16:40) 浙江大学	Carleman estimate and applications for piezoelectric equations
张磊 (HLJU) (16:40-17:00) 黑龙江大学	Numerical solution of scattering and inverse scattering for rough surfaces
张海文 (17:00-17:20) 中国科学院数学与系统科学研究院	Inverse scattering problem from phaseless far-field data

S07-2 流体力学方程的数学理论和数值方法

时间: 7 月 21 日 16:20-18:00 会场: 19 号楼 2 层, 第十会议室

组织者: 汤华中(北京大学数学科学学院)

成娟(北京应用物理与计算数学研究所)

报告人	题目
蔡力 (16:20-16:40) 西北工业大学理学院应用数学系	基于 IB/LS 方法的“左心室-血液”FSI 数值模拟
陈艺冰 (16:40-17:00) 北京应用物理与计算数学研究所	基于通量分裂思想的时空高精度紧致格式
李刚 (17:00-17:20) 青岛大学数学与统计学院	浅水波方程的基于静水重构的间断 Galerkin 方法
袁海专 (17:20-17:40) 湘潭大学数学与计算科学学院	A free energy-based surface tension force model for simulation of multiphase flows by level-set method
钟杏慧 (17:40-18:00) 浙江大学数学科学学院	Compact WENO Limiters for Discontinuous Galerkin Methods

S08-2 无界域数学物理方程的数值方法及其应用

时间: 7 月 21 日 16:20-18:00 会场: 19 号楼 2 层, 第九会议室

组织者: 武海军(南京大学)

张继伟(北京计算科学研究中心)

郑春雄(清华大学)

报告人	题目
赖俊 (16:20-16:40) 浙江大学数学科学学院	Robust integral formulations for electromagnetic scattering from three-dimensional cavities
李步扬 (16:40-17:00) 香港理工大学数学系	A-stable time discretizations preserves maximal parabolic regularity
陆雅言 (17:00-17:20) 香港城市大学数学系	Asymptotic boundary conditions for periodic waveguides
邵嗣烘 (17:20-17:40) 北京大学数学科学学院	无界区域非线性 Dirac 孤波的计算及稳定性分析

S11-2 最优化专题**时间:** 7 月 21 日 16:20-18:00 **会场:** 12 号楼 2 层, 第一会议室**组织者:** 戴戡虹(中国科学院数学与系统科学研究院)

杨庆之(中国科学院数学与系统科学研究院)

报告人	题目
蔡邢菊 (16:20-16:40) 南京师范大学	Nonnegative Tensor Factorizations Using an Alternating Direction Method
白敏茹 (16:40-17:00) 湖南师范大学	A descent cautious BFGS method for computing US-eigenvalues of symmetric complex tensors
魏益民 (17:00-17:20) 复旦大学	张量最佳秩一逼近的神经网络算法

S13-2 生命科学中的计算数学**时间:** 7 月 21 日 16:20-18:00 **会场:** 19 号楼 2 层, 第五会议室**组织者:** 李铁军(北京大学)

周栋焯(上海交通大学)

报告人	题目
张磊 (16:20-16:40) 北京大学	Phase field modeling of Cell Polarity and Cell Delamination
李铁军 (16:40-17:00) 北京大学	Inferring biological networks with strong associations by information theoretic approaches
周栋焯 (17:00-17:20) 上海交通大学	A probability polling state of neuronal systems underlying maximum entropy coding principle

T01-2 微分方程数值计算及应用**时间:** 7月21日 16:20-18:00 **会场:** 10号楼6层, 第一会议室**主持人:** 刘雪娇(中国科学院数学与系统科学研究院)

王涵(北京应用物理与计算数学研究所)

倪冉(Nanyang Technological University)

报告人	题目
王涵 (16:20-16:40) 北京应用物理与计算数学研究所	The equilibrium melting path of the hexagonal ice.
倪冉 (16:40-16:55) Nanyang Technological University	Glassy dynamics, spinodal fluctuations, and the kinetic limit of nucleation in suspensions of colloidal hard rods
刘雪娇 (16:55-17:10) 中国科学院数学与系统科学研究院	应用 Born 自能修正的 Poisson-Nernst-Planck 模型研究 Kcsa 钾离子通道的选择性

T03-2 优化、控制及反问题**时间:** 7月21日 16:20-18:00 **会场:** 19号楼2层, 第二会议室**主持人:** 张永金(河南理工大学)

徐英祥(东北师范大学数学与统计学院)

郭双冰(河南科技学院)

报告人	题目
徐英祥 (16:20-16:40) 东北师范大学数学与统计学院	Optimized Schwarz methods for the optimal control of systems governed by elliptic partial differential equations
郭双冰 (16:40-16:55) 河南科技学院	The Eigenvalue Optimization Problem in Quantum Dots
张永金 (16:55-17:10) 河南理工大学	An efficient error estimation for model order reduction of parametrized evolution equations

T05-1 谱方法、数值逼近与计算几何**时间:** 7 月 21 日 16:20-18:00 **会场:** 19 号楼 2 层, 第三会议室**主持人:** 李金(山东建筑大学)

王同科(天津师范大学数学科学学院)

吴善和(龙岩学院)

报告人	题目
王同科 (16:20-16:40) 天津师范大学数学科学学院	A robust algorithm for the inversion of Laplace transform using Puiseux expansion
吴善和 (16:40-17:00) 龙岩学院	Fast convergence of generalized DeTemple sequences and the relation to the Zeta function
李金 (17:00-17:20) 山东建筑大学	一类二维 Cauchy 主值积分的近似计算
王敏 (17:20-17:35) 复旦大学	A Further Analysis of Backward Error in Polynomial Deflation
翟佳音 (17:35-17:50) 南京师范大学	Fractional Hermite Interpolation Formulas for Non-smooth Functions

T06-2 有限元和边界元方法**时间:** 7 月 21 日 16:20-18:00 **会场:** 12 号楼 3 层, 第三会议室**主持人:** 冯春生(湘潭大学)

董巧丽(中国民航大学)

夏银华(中国科学技术大学)

报告人	题目
董巧丽 (16:20-16:40) 中国民航大学	Multi-step inertial Krasnoselskii-Mann algorithm for nonexpansive mappings
夏银华 (16:40-17:00) 中国科学技术大学	Arbitrary Lagrangian-Eulerian discontinuous Galerkin method for conservation laws
冯春生 (17:00-17:20) 湘潭大学	一种求解三维 Neumann 边界条件线弹性问题线性二次有限元方程的并行高效预条件子
张进 (17:20-17:35) 山东师范大学	SDFEMs on Triangular Meshes for Convection-dominated Problems
张百驹 (17:35-17:50) 四川大学数学学院	Virtual Element Method for Linear Elasticity Problem in Mixed Weakly Symmetric Formulation

T09-2 分数阶方程**时间:** 7 月 21 日 16:20-18:00 **会场:** 10 号楼 6 层, 第二会议室**主持人:** 杨雪花(北京计算物理与应用数学研究所)

蔡好涛(山东财经大学)

任金城(河南财经政法大学)

报告人	题目
蔡好涛 (16:20-16:40) 山东财经大学	A Fractional Order Collocation Method for Second Kind Volterra Integral Equations with Weakly Singular Kernels
任金城 (16:40-17:00) 河南财经政法大学	Fast evaluation and high accuracy finite element approximation for the time fractional subdiffusion equation
杨雪花 (17:00-17:15) 北京计算物理与应用数学研究所	Orthogonal spline collocation method for fourth-order fractional evolution equation
张海湘 (17:15-17:30) 湖南工业大学	The extrapolated Crank-Nicolson OSC method for a nonlinear fractional Cable equation with nonlinear variable coefficient
黄朝宝 (17:30-17:45) 北京计算科学研究中心	Optimal error analysis of a direct discontinuous Galerkin method for time-fractional reaction-diffusion equation
郝朝鹏 (17:45-18:00) 东南大学数学学院	Regularity and spectral methods for two-sided fractional differential equations with a low order

分会场报告 3

S01-1 PDE 并行、快速算法研究进展

时间：7月22日 14:00-16:00 会场：12号楼2层，第一会议室

组织者：蔡小川(中国科学院深圳先进技术研究院, *University of Colorado Boulder*)

黄记祖(中国科学院数学与系统科学研究院科学与工程计算研究所)

陈荣亮(中国科学院深圳先进技术研究院)

报告人	题目
刘杰 (14:00-14:20) 国防科学技术大学	非结构网格粒子输运问题的并行计算
张玉 (14:20-14:40) 西安电子科技大学	计算电磁学中矩量法的复数稠密矩阵方程问题研究
徐小文 (14:40-15:00) 北京应用物理与计算数学研究所	面向复杂应用数值模拟的自适应预条件策略
杨自豪 (15:00-15:20) 西北工业大学	具有多重小周期构造的复合材料结构热传导问题的高阶三尺度方法
盛志强 (15:20-15:40) 北京应用物理与计算数学研究所	热传导方程的并行有限体积格式

S03-1 界面问题的建模与计算**时间:** 7 月 22 日 14:00-16:00 **会场:** 19 号楼 2 层, 第四会议室**组织者:** 邸亚娜(中国科学院数学与系统科学研究院)

于海军(中国科学院数学与系统科学研究院)

许现民(中国科学院数学与系统科学研究院)

报告人	题目
张辉 (14:00-14:20) 北京师范大学	Invariant Energy Quadratization Approach for Incompressible Smectic-A Liquid Crystal Flow
徐岩 (14:20-14:40) 中国科学技术大学	High order energy stable and efficient local discontinuous Galerkin methods for the phase field models
杨将 (14:40-15:00) 美国哥伦比亚大学	Efficient and accurate Fourier approximations of nonlocal phase-field equations
郑伟英 (15:00-15:20) 中国科学院数学与系统科学研究院	三维理想 MHD 方程的严格 divergence-free 非结构网格 DG 方法
蔡勇勇 (15:20-15:40) 北京计算科学研究中心	Error estimates for a fully discretized scheme to a Cahn-Hilliard phase-field model for two-phase incompressible flows
季霞 (15:40-16:00) 中国科学院数学与系统科学研究院	Recursive Integral Method For The Nonlinear Non-Selfadjoint Transmission Eigenvalue Problem

S04-1 材料科学的可计算建模与计算方法**时间:** 7月22日 14:00-16:00 **会场:** 19号楼2层, 第三会议室**组织者:** 高兴誉(北京应用物理与计算数学研究所)

王涵(北京应用物理与计算数学研究所)

报告人	题目
陈景润 (14:00-14:20) 苏州大学	Density Functional Theory: Two Cases Study
刘芳 (14:20-14:40) 中央财经大学	An efficient algorithm for the Sternheimer equation in the GW approximation
张鉴 (14:40-15:00) 中国科学院计算机网络信息中心	Extreme-Scale Phase Field Simulations of Coarsening Dynamics on the Sunway TaihuLight Supercomputer
邵嗣烘 (15:00-15:20) 北京大学	Deterministic Solvers for the Wigner Quantum Dynamics
王皓 (15:20-15:40) 四川大学	Atomistic-to-continuum coupling method and its adaptivity
胡光辉 (15:40-16:00) 澳门大学	On adaptive finite element simulations of high harmonic generation with time-dependent density functional theory

S05-1 Recent advances in nonstandard discretization methods in scientific and engineering computation

时间: 7月22日 14:00-16:00 会场: 19号楼2层, 第十会议室

组织者: 胡俊(北京大学)

谢小平(四川大学)

徐立伟(电子科技大学)

张然(吉林大学)

报告人	题目
崔金涛 (14:00-14:20) 香港理工大学	A nonconforming finite element method for an acoustic fluid-structure interaction problem
黄建国 (14:20-14:40) 上海交通大学	An optimal high-order locking-free finite element method for elastic vibration problems
黄学海 (14:40-15:00) 温州大学	Differential complex, Hemioltz decompositions and mixed methods
汪艳秋 (15:00-15:20) 南京师范大学	A nonconforming finite element on polygonal meshes
王坤 (15:20-15:40) 重庆大学	Efficient and accurate numerical solutions for the Helmholtz equation with high wave numbers
吴永科 (15:40-16:00) 电子科技大学	Convergence of adaptive mixed finite element methods for Hodge Laplacian wquation: without harmonic forms

S09-1 Krylov 子空间算法及预处理技术**时间:** 7 月 22 日 14:00-16:00 **会场:** 19 号楼 2 层, 第二会议室**组织者:** 顾先明(电子科技大学数学科学学院)

报告人	题目
殷俊峰 (14:00-14:20) 同济大学数学科学学院	Preconditioned modified Hermitian and skew-Hermitian splitting iteration methods for the fractional nonlinear Schrödinger equations
吴钢 (14:20-14:40) 中国矿业大学数学学院	A weighted global GMRES method with deflation for solving linear Sylvester equations
李铁香 (14:40-15:00) 东南大学数学学院	Efficient numerical algorithms for computing positive interior transmission eigenvalues
牛强 (15:00-15:20) 西交利物浦大学数学科学系	Analysis of a new dimension-wise splitting iteration with selective relaxation for saddle point problems
张建华 (15:20-15:40) 东华理工大学数学系	A new iterative method for solving complex symmetric linear systems
顾先明 (15:40-16:00) 电子科技大学数学科学学院	Inner-outer iterative variants of the CMRH method for solving multi-shifted non-Hermitian linear systems

T01-3 微分方程数值计算及应用**时间:** 7 月 22 日 14:00-16:00 **会场:** 10 号楼 6 层, 第一会议室**主持人:** 余翌帆(中国科学院数学与系统科学研究院)

崔霞(北京应用物理与计算数学研究所)

常静雅(香港理工大学)

报告人	题目
崔霞 (14:00-14:20) 北京应用物理与计算数学研究所	非平衡辐射扩散问题的渐近保持数值模拟
常静雅 (14:20-14:40) 香港理工大学	Computing the p-Spectral Radii of Uniform Hypergraphs with Applications
余翌帆 (14:40-14:55) 中国科学院数学与系统科学研究院	基于 BCC/FCC 晶格的金属材料微观力学行为分析
马召灿 (14:55-15:10) 中科院计算数学所	3D Simulation of the Defect Generation by Hydrogen at $Si - SiO_2$ Interface
朱湘疆 (15:10-15:25) 北京大学	一类含奇异项的微分积分方程的适定性理论及其在稳态 Wigner 方程中的应用

T06-3 有限元和边界元方法**时间:** 7 月 22 日 14:00-16:00 **会场:** 12 号楼 3 层, 第三会议室**主持人:** 宋伦继(兰州大学)

沈晓芹(西安理工大学)

黄佩奇(南京林业大学)

报告人	题目
沈晓芹 (14:00-14:20) 西安理工大学	The time-dependent flexural shell model and its numerical simulations
黄佩奇 (14:20-14:40) 南京林业大学	A Partially Penalized Immersed Interface Finite Element Method for Planar Elasticity Interface Problems
宋伦继 (14:40-15:00) 兰州大学	A Weak Galerkin Method with an Over-Relaxed Stabilization for Low Regularity Elliptic Problems
赵纪坤 (15:00-15:15) 郑州大学	Nonconforming virtual element method for plate bending problems
王疆兴 (15:15-15:30) 北京计算科学研究中心	Error estimate of CGDG method and its fast evaluation for Maxwell's equations in Cole-Cole dispersive media
许竞劼 (15:30-15:45) 中国科学院数学与系统科学研究院	Enzyme and Nanopore Simulations by Finite Element Method

T07-1 多重网格技术、区域分解及并行计算**时间:** 7 月 22 日 14:00-16:00 **会场:** 19 号楼 2 层, 第九会议室**主持人:** 岳孝强(湘潭大学)

姚彦忠(北京应用物理与计算数学研究所)

刘会坡(北京应用物理与计算数学研究所)

报告人	题目
姚彦忠 (14:00-14:25) 北京应用物理与计算数学研究所	An efficient parallel iteration algorithm for radiation diffusion equation
刘会坡 (14:25-14:45) 北京应用物理与计算数学研究所	Superconvergence two-grid scheme based on shifted-inverse power method for eigenvalue problems by function value recovery
岳孝强 (14:45-15:00) 湘潭大学	Substructuring Preconditioners with a Simple Coarse Space for 2-D 3-T Radiation Diffusion Equations
袁龙 (15:00-15:15) 山东科技大学	并行求解平面波 Helmholtz 和 Maxwell 离散系统
徐飞 (15:15-15:30) 北京工业大学	A Parallel Multigrid Method For Semilinear Elliptic Equation
黄健 (15:30-15:45) 山东大学	Multigrid Methods for A Mixed Finite Element Method of The Darcy-Forchheimer Model
董丽秀 (15:45-16:00) 北京师范大学	Convergence Analysis and Numerical Implementation of a Second Order Numerical Scheme for the Three-Dimensional Phase Field Crystal Equation

T09-3 分数阶方程**时间:** 7月22日 14:00-16:00 **会场:** 10号楼6层, 第二会议室**主持人:** 李步扬(*The Hong Kong Polytechnic University*)

曹婉容(东南大学)

阮周生(东华理工大学)

报告人	题目
曹婉容 (14:00-14:20) 东南大学	Implicit-Explicit difference schemes for nonlinear fractional differential equations with smooth inputs
阮周生 (14:20-14:40) 东华理工大学	Simultaneous inversion of the fractional order and the space-dependent source term for the time-fractional diffusion equation
李步扬 (14:40-15:00) <i>The Hong Kong Polytechnic University</i>	High-order BDF convolution quadrature for fractional evolution equations
赵旭鹰 (15:00-15:15) 中科院数学与系统科学研究院	Quantitative dependence analysis on the horizon for nonlocal diffusion models
周知 (15:15-15:30) 香港理工大学	时间分数阶扩散方程高精度数值格式的修正
王冬岭 (15:30-15:50) 西北大学	Asymptotic behaviours and numerical approximations for F-ODEs and F-FDEs

分会场报告 4

S01-2 PDE 并行、快速算法研究进展

时间: 7 月 22 日 16:20-18:00 会场: 12 号楼 2 层, 第一会议室

组织者: 蔡小川(中国科学院深圳先进技术研究院, *University of Colorado Boulder*)

黄记祖(中国科学院数学与系统科学研究院科学与工程计算研究所)

陈荣亮(中国科学院深圳先进技术研究院)

报告人	题目
罗力 (16:20-16:40) 中国科学院深圳先进技术研究院	A parallel finite element method for 3D moving contact line problem in complex domain with applications
王锋 (16:40-17:00) 南京师范大学	A divergence free virtual element method for the Stokes problem on polyhedral meshes
闫争争 (17:00-17:20) 中国科学院深圳先进技术研究院	A Domain Decomposition Based Method for the Simulation of Wind Flows over Large Urban Areas
李世顺 (17:20-17:40) 河南理工大学	Introduction of some space-time Schwarz algorithms for parabolic equation

S03-2 界面问题的建模与计算

时间: 7 月 22 日 16:20-18:00 会场: 19 号楼 2 层, 第四会议室

组织者: 邸亚娜(中国科学院数学与系统科学研究院)

于海军(中国科学院数学与系统科学研究院)

许现民(中国科学院数学与系统科学研究院)

报告人	题目
应文俊 (16:20-16:40) 上海交通大学	A Cartesian grid method for moving interface problems
蒋维 (16:40-17:00) 武汉大学	A parametric finite element method for solid-state dewetting problems with anisotropic surface energies
王何宇 (17:00-17:20) 浙江大学	自由表面问题的混合元方法及其快速算子
许现民 (17:20-17:40) 中国科学院数学与系统科学研究院	Use Onsager Principle as an approximation tool in some liquid problems with moving interfaces

S04-2 材料科学的可计算建模与计算方法**时间:** 7月22日 16:20-18:00 **会场:** 19号楼2层, 第三会议室**组织者:** 高兴誉(北京应用物理与计算数学研究所)

王涵(北京应用物理与计算数学研究所)

报告人	题目
阳莺 (16:20-16:40) 桂林电子科技大学	Poission-Nernst-Planck 方程的两网格有限元计算
李胜国 (16:40-17:00) 国防科学技术大学	一种求解特征值和奇异值的新型分布式并行算法
潘妍 (17:00-17:20) 中国科学院数学与系统科学研究院	基于平面波离散的并行轨道更新方法新进展
张力维 (17:20-17:40) 中国科学院数学与系统科学研究院	电子结构计算的保正交共轭梯度法
高兴誉 (17:40-18:00) 北京应用物理与计算数学研究所	The preconditioning function for the linearized DFT eigenvalue problem with plane wave basis

S05-2 Recent advances in nonstandard discretization methods in scientific and engineering computation

时间: 7 月 22 日 16:20-18:00 会场: 19 号楼 2 层, 第十会议室

组织者: 胡俊(北京大学)

谢小平(四川大学)

徐立伟(电子科技大学)

张然(吉林大学)

报告人	题目
谢和虎 (16:20-16:40) 中国科学院计算数学研究所	非协调有限元特征值问题的多重网格算法
谢小平 (16:40-17:00) 四川大学	Regularity for time fractional wave problems
张然 (17:00-17:20) 吉林大学	Maximum principles for P1-P0 weak Galerkin finite element approximations of quasi-linear Second order elliptic equations
张世全 (17:20-17:40) 四川大学	The optimal EDG methods and fast solvers for the general diffusion problems
张硕 (17:40-18:00) 中国科学院计算数学研究所	Order reduced methods for fourth order problems

S08-3 无界域数学物理方程的数值方法及其应用**时间:** 7月22日 16:20-18:00 **会场:** 19号楼2层, 第九会议室**组织者:** 武海军(南京大学)

张继伟(北京计算科学研究中心)

郑春雄(清华大学)

报告人	题目
武海军 (16:20-16:40) 南京大学数学系	FEM and CIP-FEM for Helmholtz Equation with High Wave Number and PML truncation
徐立伟 (16:40-17:00) 电子科技大学数学学院	Boundary integral equation methods for acoustic and elastic waves
应文俊 (17:00-17:20) 上海交通大学自然科学研究院	An efficient adaptive rescaling scheme for computing moving interface problems
张磊 (17:20-17:40) 北京大学工学院	无界域空间半离散波动方程的人工边界条件及稳定性分析
郑伟英 (17:40-18:00) 中国科学院数学与系统科学研究院	Perfectly matched layer method for electromagnetic scattering problems in layered media

T02-3 流体力学中的数值计算**时间:** 7 月 22 日 16:20-18:00 **会场:** 10 号楼 6 层, 第一会议室**主持人:** 王晓东(西北工业大学)

曾清红(北京应用物理与计算数学研究所)

沈智军(北京应用物理与计算数学研究所)

报告人	题目
曾清红 (16:20-16:40) 北京应用物理与计算数学研究所	复杂构型流动问题的多介质 ALE 模拟
沈智军 (16:40-17:00) 北京应用物理与计算数学研究所	健壮的流体力学一维形式黎曼解
王晓东 (17:00-17:20) 西北工业大学	流动诱导聚合物结晶的建模与模拟
龚跃政 (17:20-17:35) 北京计算科学研究中心	Linear Energy Stable Scheme for Quasi-incompressible Hydrodynamic Binary Fluid Model
孔慧慧 (17:35-17:50) 北京计算科学研究中心	Free boundary value problem to 3D spherically symmetric compressible Navier–Stokes–Poisson equations

T05-2 谱方法、数值逼近与计算几何**时间:** 7月22日 16:20-18:00 **会场:** 19号楼2层, 第二会议室**主持人:** 刘飞(华中科技大学)

安静(北京计算科学研究中心)

李昭祥(上海师范大学数学系)

报告人	题目
安静 (16:20-16:40) 北京计算科学研究中心	An efficient spectral-Galerkin approximation and error analysis for Maxwell transmission eigenvalue problems in spherical geometries
李昭祥 (16:40-17:00) 上海师范大学数学系	Pseudospectral methods for computing the multiple solutions of the Schrodinger equation
刘飞 (17:00-17:15) 华中科技大学	A MATLAB-based Fourier-Spectral Solver for Phase-Field Simulations
廖锋 (17:15-17:30) 南京航空航天大学	Time splitting-exponential wave integrator Fourier pseudospectral method for Schrödinger-Boussinesq system
刘伟 (17:30-17:45) 湖南师范大学	Finding Excited States of Bose-Einstein Condensates by a Constrained Gentlest Ascent Dynamics
高天成 (17:45-18:00) 北京航空航天大学	A local-adjustment based two-dimensional Delaunay triangular mesh generation method on a bounded domain with moving boundary

T06-4 有限元和边界元方法**时间:** 7 月 22 日 16:20-18:00 **会场:** 12 号楼 3 层, 第三会议室**主持人:** 魏华祎(湘潭大学)

姚昌辉(郑州大学)

黄红英(浙江海洋大学)

报告人	题目
姚昌辉 (16:20-16:40) 郑州大学	非线性电磁场方程的全离散 $A-\varphi$ 有限元方法
黄红英 (16:40-17:00) 浙江海洋大学	Staggered discontinuous Galerkin method for P-Stokes systems
魏华祎 (17:00-17:20) 湘潭大学	Array-oriented Finite Element Method Programming in Python
王梦莹 (17:20-17:35) 北京航空航天大学	The effect of mesh geometry on the condition number of stiffness matrix of finite element for Plate Bending Problems
马利敏 (17:35-17:50) 北京大学	Penalized Crouzeix-Raviart method for eigenvalue problems

T09-4 分数阶方程**时间:** 7月22日 16:20-18:00 **会场:** 10号楼6层, 第二会议室**主持人:** 孟祥云(北京计算科学研究中心)

闫玉斌(英国切斯特大学(吕梁学院特聘))

祁瑞生(东北大学秦皇岛分校)

报告人	题目
闫玉斌 (16:20-16:40) 英国切斯特大学(吕梁学院特聘)	An analysis of the modified L1 scheme for the time-fractional partial differential equations with nonsmooth data
祁瑞生 (16:40-16:55) 东北大学秦皇岛分校	Sharper error bound for a discontinuous Galerkin, time-stepping method for a fractional stochastic diffusion equation disturbed by fraction Brownian motions
孟祥云 (16:55-17:10) 北京计算科学研究中心	A sharp maximum principle for a two-point boundary value problem with a Caputo fractional derivative
张治江 (17:10-17:25) 兰州大学	Numerical approaches to the functional distribution of anomalous diffusion with both traps and flights
李猛 (17:25-17:40) 华中科技大学	Two conservative finite element schemes for the strongly coupled nonlinear fractional Schrodinger equations
纪翠翠 (17:40-17:55) 东南大学	The analysis of stability and convergence of the numerical scheme for the time-fractional sub-diffusion equation with non-local boundary conditions

分会场报告 5

S10-1 有限体积法理论及其应用

时间: 7 月 23 日 14:00-16:00 会场: 12 号楼 2 层, 第一会议室

组织者: 邹青松(中山大学)

李永海(吉林大学)

报告人	题目
林延平 (14:00-14:20) 香港理工大学	Linear and Quadratic Immersed Finite Element Methods for the Multilayer Porous Wall Model
邹青松 (14:20-14:40) 中山大学	On the locally conserving flux derived from a finite element solution
王翔 (14:40-14:55) 吉林大学	L^2 error estimate and superconvergence of high order finite volume methods on triangular meshes
邬吉明 (14:55-15:15) 北京应用物理与计算数学研究所	A family of vertex-centered linearity-preserving schemes for diffusion problems on arbitrary polygonal meshes
张志跃 (15:15-15:35) 南京师范大学	Energy-Preserving Finite Volume Element Method for the Boussinesq equations

S12-1 稀有事件及其鞍点问题的计算与应用**时间:** 7 月 23 日 14:00-16:00 **会场:** 19 号楼 2 层, 第二会议室**组织者:** 张磊(北京大学)

任维清(新加坡国立大学)

杨志坚(武汉大学)

报告人	题目
周翔 (14:00-14:20) 香港城市大学	Theoretical and Numerical Advancement for Transition State Calculations in Rare-event Study
李铁军 (14:20-14:40) 北京大学	芽殖酵母细胞周期 S 期检验点激活的稀有事件研究
汪涵 (14:40-15:00) 北京应用物理与计算数学研究所	The equilibrium melting path of the hexagonal ice
于海军 (15:00-15:20) 中科院计算数学所	Convergence Analysis of a Minimum Action Method for Non-gradient Systems
Ran NI (15:20-15:40) Nanyang Technological University	Glassy dynamics, spinodal fluctuations, and the kinetic limit of nucleation in suspensions of colloidal hard rods

T02-1 流体力学中的数值计算**时间:** 7 月 23 日 14:00-16:00 **会场:** 19 号楼 2 层, 第十会议室**主持人:** 徐骁(北京应用物理与计算数学研究所)

黄鹏展(新疆大学数学与系统科学学院)

许晓阳(陕西理工大学)

报告人	题目
黄鹏展 (14:00-14:20) 新疆大学数学与系统科学学院	Second order time-space iterative method for the stationary Navier-Stokes equations
许晓阳 (14:20-14:40) 陕西理工大学	溃坝流问题的改进 SPH 方法模拟
徐骁 (14:40-14:55) 北京应用物理与计算数学研究所	不同三维网格下的拉氏流体数值分析
陈锐 (14:55-15:10) 北京应用物理与计算数学研究所	Linear, Second Order and Unconditionally Energy Stable Schemes for a hydrodynamic model of Smectic-A Liquid Crystals
曹雅茹 (15:10-15:30) 北京航空航天大学	An efficient exponential integrator factor method with non-polynomial direct discontinuous Galerkin spatial approximation for solving viscous Burgers' equations
王华 (15:30-15:45) 南京师范大学	Enriched Finite Element Methods for Stokes Interface Problems
赵立飞 (15:45-16:00) 西北工业大学	粘弹性流动问题非结构网格有限体积法的高效求解

T04-1 数值代数**时间:** 7 月 23 日 14:00-16:00 **会场:** 10 号楼 6 层, 第一会议室**主持人:** 吴庆标(浙江大学数学科学学院)

白正简(厦门大学)

高卫国(复旦大学)

报告人	题目
白正简 (14:00-14:20) 厦门大学	A Riemannian Newton Method for Nonnegative Inverse Eigenvalue Problems
高卫国 (14:20-14:40) 复旦大学	Jacobi-Like Algorithm for Bethe-Salpeter Eigenvalue Problem
吴庆标 (14:40-15:00) 浙江大学数学科学学院	Multi-step modified Newton-NSS method for solving systems of nonlinear equations
卢欣 (15:00-15:15) 中国石油大学 (北京)	The convergence theory for the restricted version of the overlapping Schur complement preconditioner
郭培昌 (15:15-15:30) 中国地质大学 (北京)	Markovian 二叉树中二次向量方程的算法
张瑞 (15:30-15:45) 湖南师范大学	GMRES Method for Multi-Scattering Problems
王会迪 (15:45-16:00) 浙江大学数学科学学院	On a simpler SSOR-like method for augmented systems

T06-5 有限元和边界元方法**时间:** 7 月 23 日 14:00-16:00 **会场:** 10 号楼 6 层, 第二会议室**主持人:** 王淑琴(西北工业大学)

王飞(西安交通大学)

葛志昊(河南大学)

报告人	题目
王飞 (14:00-14:20) 西安交通大学	Virtual Element Methods for Obstacle Problem
葛志昊 (14:20-14:40) 河南大学	多孔弹性模型多物理场有限元方法
王淑琴 (14:40-14:55) 西北工业大学	Navier-Stokes 方程: 局部间断 Galerkin 方法, 非线性稳定性, 收敛性。
王海金 (14:55-15:10) 南京邮电大学	Local discontinuous Galerkin methods with implicit-explicit time-marching for time-dependent incompressible fluid flow

T08-1 自适应方法**时间:** 7 月 23 日 14:00-16:00 **会场:** 12 号楼 3 层, 第三会议室**主持人:** 吕俊良(吉林大学)

朱洪强(南京邮电大学)

龚伟(中科院数学与系统科学研究院)

报告人	题目
朱洪强 (14:00-14:20) 南京邮电大学	An h -adaptive RKDG method and its applications
龚伟 (14:20-14:40) 中科院数学与系统科学研究院	A Convergent Adaptive Finite Element Method for Elliptic Dirichlet Boundary Control Problems
吕俊良 (14:40-15:00) 吉林大学	Adaptive finite element methods for scattering problems in unbounded domain
刘利斌 (15:00-15:15) 广西师范学院	A parameter-uniform adaptive grid method for singularly perturbed parabolic convection-diffusion problems
王利娜 (15:15-15:30) 上海师范大学	An h - p Version Of The Continuous Petrov-Galerkin Method For Volterra Delay-Integro-Differential Equations

T10-1 随机微分方程**时间:** 7 月 23 日 14:00-16:00 **会场:** 19 号楼 2 层, 第四会议室**主持人:** 郭谦(上海师范大学)

徐承龙(同济大学)

姜立建(湖南大学)

报告人	题目
徐承龙 (14:00-14:20) 同济大学	Hybrid Monte Carlo Acceleration Method for Pricing European Options under Levy Processes
姜立建 (14:20-14:40) 湖南大学	Variable-separation methods based on sparse and low rank representation for stochastic partial differential equations
郭谦 (14:40-15:00) 上海师范大学	超线性随机微分方程的数值方法
袁海燕 (15:00-15:20) 黑龙江工程学院	Mean square stability of semi-implicit Euler method for non-linear neutral stochastic delay integro differential equations
付余 (15:20-15:35) 山东科技大学	Generator approximation method for solving forward backward stochastic differential equations and its applications
逯伯亮 (15:35-15:50) 南京财经大学	Stability of a class of hybrid stochastic neutral differential equations with unbounded delay
刘永乐 (15:50-16:05) 上海师范大学	Stochastic Collocation via nonconvex compressive sensing and its application to solve SPDEs with random inputs

T11-1 有限差分法及其应用**时间:** 7 月 23 日 14:00-16:00 **会场:** 19 号楼 2 层, 第三会议室**主持人:** 高理平(中国石油大学(华东)理学院)

杭旭登(北京应用物理与计算数学研究所)

冯秀芳(宁夏大学)

报告人	题目
杭旭登 (14:00-14:20) 北京应用物理与计算数学研究所	三维扩散方程的金字塔格式
冯秀芳 (14:20-14:40) 宁夏大学	求解带有不连续系数和非奇异源项的 Helmholtz 方程的高阶紧致格式
高理平 (14:40-15:00) 中国石油大学(华东)理学院	Energy conservation and super convergence analysis of the EC-S-FDTD method for Maxwell equations with periodic boundaries
钱旭 (15:00-15:15) 国防科学技术大学	Conservative modified Crank–Nicolson and time-splitting wavelet methods for modeling Bose–Einstein condensates in delta potentials
王姗姗 (15:15-15:30) 南京航空航天大学	Some numerical researches on split-step methods
周旋旋 (15:30-15:45) 南京航空航天大学	conservative compact difference scheme for the zakharov equaiton
鲜双燕 (15:45-16:00) 宁夏大学	求解三维变系数 Helmholtz 方程的高阶紧致差分格式

T12-1 移动网格和无网格及有限体积法**时间:** 7 月 23 日 14:00-16:00 **会场:** 19 号楼 2 层, 第九会议室**主持人:** 彭洁(湘潭大学)

李小林(重庆师范大学)

冯仁忠(北京航空航天大学)

报告人	题目
李小林 (14:00-14:20) 重庆师范大学	Analysis of two moving least squares approximation-based meshless methods
冯仁忠 (14:20-14:40) 北京航空航天大学	基于径向基函数插值的高精度差商及其在微分方程求解中的应用
彭洁 (14:40-14:55) 湘潭大学	Eulerian 网格下含内界面的定常扩散问题的一种有限体积格式的误差估计
张齐 (14:55-15:10) 中国工程物理研究院研究生院	A monotone finite volume scheme for diffusion equations on general non-conforming meshes

分会场报告 6**S01-3 PDE 并行、快速算法研究进展****时间:** 7 月 23 日 16:20-18:00 **会场:** 19 号楼 2 层, 第三会议室**组织者:** 蔡小川(中国科学院深圳先进技术研究院, *University of Colorado Boulder*)

黄记祖(中国科学院数学与系统科学研究院科学与工程计算研究所)

陈荣亮(中国科学院深圳先进技术研究院)

报告人	题目
蔡小川 (16:20-16:40) 中国科学院深圳先进技术研究院, <i>University of Colorado Boulder</i>	Nonlinearly Preconditioned Newton's Methods for PDEs
黄记祖 (16:40-17:00) 中国科学院数学与系统科学研究院 科学与工程计算研究所	基于格子 Boltzmann 模型的两相流数值模拟
徐磊 (17:00-17:20) 上海大学	Finite Volume Lattice Boltzmann Method for High Mach Compressible Flows on Unstructured Meshes

S10-2 有限体积法理论及其应用

时间: 7 月 23 日 16:20-18:00 会场: 12 号楼 2 层, 第一会议室

组织者: 邹青松(中山大学)

李永海(吉林大学)

报告人	题目
何文明 (16:20-16:40) 温州大学	高次有限元方法的后处理算法
曹外香 (16:40-17:00) 中山大学	Superconvergence of Immersed Finite Volume Methods for Interface Problems
刘玉洁 (17:00-17:20) 中山大学	Cell-centered finite volume element methods for elliptic equations
张庆辉 (17:20-17:40) 中山大学	Generalized Finite Volume Methods for Elliptic Interface Problems
高志明 (17:40-18:00) 北京应用物理与计算数学研究所	A Posteriori Error Estimates for Cell Functional Minimization Scheme Applied to Elliptic Equations

S12-2 稀有事件及其鞍点问题的计算与应用

时间: 7 月 23 日 16:20-18:00 会场: 19 号楼 2 层, 第二会议室

组织者: 张磊(北京大学)

任维清(新加坡国立大学)

杨志坚(武汉大学)

报告人	题目
张亚楠 (16:20-16:40) 苏州大学	Numerical Study of the Effects of Surface Topography and Chemistry on the Wetting Transition Using the String method
靳聪明 (16:40-17:00) 浙江理工大学	The Application of the String method to the Dislocation Dynamics
张磊 (17:00-17:20) 北京大学	Recent Developments in Numerical Methods of Finding Saddle Points and its Applications in Materials

T02-2 流体力学中的数值计算**时间:** 7月23日 16:20-18:00 **会场:** 19号楼2层, 第十会议室**主持人:** 彭秋瑾(中国人民大学)

李义宝(西安交通大学)

叶挺(吉林大学)

报告人	题目
李义宝 (16:20-16:40) 西安交通大学	A phase-field fluid modeling and computation with interfacial profile correction term
叶挺 (16:40-17:00) 吉林大学	A Hybrid Smoothed Dissipative Particle Dynamics and Immersed Boundary method (SDPD-IBM) for Simulation of Red Blood Cells (RBCs) in Flows
彭秋瑾 (17:00-17:15) 中国人民大学	The Phase Transition Model for Heat-Shrinkable Thermo-Sensitive Hydrogels Based on Interaction Energy
徐真 (17:15-17:30) 北京师范大学	Error estimates for the decoupled, energy stable schemes for Cahn-Hilliard Phase-field models of two-phase incompressible flows
李晓丽 (17:30-17:45) 山东大学	Characteristic block-centered finite difference method for simulating incompressible wormhole propagation
赵刚 (17:45-18:00) 中国科学院数学与系统科学研究院	Moving Staggered Mesh

T04-2 数值代数**时间:** 7月23日 16:20-18:00 **会场:** 10号楼6层, 第一会议室**主持人:** 杨畅(哈尔滨工业大学)

吕长青(枣庄学院)

杜魁(厦门大学)

报告人	题目
吕长青 (16:20-16:40) 枣庄学院	An iterative scheme for identifying general H-tensor
杜魁 (16:40-17:00) 厦门大学	Ritz and harmonic Ritz values and the convergence of GM-RES
杨畅 (17:00-17:15) 哈尔滨工业大学	Iterative solvers for elliptic problems with arbitrary anisotropy strengths
吴静 (17:15-17:30) 西安思源学院	一类五对角矩阵的特征值反问题及应用
李凌霄 (17:30-17:45) 中国科学院数学与系统科学研究院	Effect Block Preconditioning for the Stationary MHD equations in 3D

T08-2 自适应方法**时间:** 7月23日 16:20-18:00 **会场:** 12号楼3层, 第三会议室**主持人:** 刘剑明(江苏师范大学)

满红英(北京理工大学)

毛士鹏(中科院计算数学所)

报告人	题目
满红英 (16:20-16:40) 北京理工大学	Residual-Based A Posteriori Error Estimates for Symmetric Conforming Mixed Finite Elements for Linear Elasticity Problems
毛士鹏 (16:40-17:00) 中科院计算数学所	Residual based a posteriori error estimates for incompressible magnetohydrodynamics
刘剑明 (17:00-17:20) 江苏师范大学	自适应笛卡尔网格方法复杂几何模拟
张蓓 (17:20-17:35) 郑州大学	A posteriori error analysis of nonconforming finite element methods for convection-diffusion problems

T09-5 分数阶方程**时间:** 7月23日 16:20-18:00 **会场:** 10号楼6层, 第二会议室**主持人:** 许传炬(厦门大学)

王宏(南卡罗来纳大学/山东大学)

徐大(湖南师范大学)

报告人	题目
王宏 (16:20-16:40) 南卡罗来纳大学/山东大学	分数阶偏微分方程的快速算法
徐大 (16:40-17:00) 湖南师范大学	Numerical solution of evolutionary integral equations with completely monotonic kernel by Runge-Kutta convolution quadrature
许传炬 (17:00-17:20) 厦门大学	Muntz Spectral Methods with Applications to Some Singular Problems
陈明华 (17:20-17:40) 兰州大学	Convergence analysis of a multigrid method for the nonlocal model

T12-2 移动网格和无网格及有限体积法**时间:** 7月23日 16:20-18:00 **会场:** 19号楼2层, 第九会议室**主持人:** 赵腾进(南京师范大学)

鲁祖亮(重庆三峡学院)

杨晓波(中国矿业大学)

报告人	题目
鲁祖亮 (16:20-16:40) 重庆三峡学院	Finite volume element method for nonlinear elliptic and parabolic optimal control problems
杨晓波 (16:40-16:55) 中国矿业大学	A moving mesh finite difference method for equilibrium radiation diffusion equations
赵腾进 (16:55-17:10) 南京师范大学	Fourier finite volume element method for Dirichlet boundary control problems governed by parabolic PDEs

五 摘要列表

冯康科学计算奖获得者报告

动理学方程的模型约化

李若¹

Abstract: 在本报告中, 我会介绍今年我们最初为玻尔兹曼方程做矩模型约化所发展起来的理论, 此理论可以应用于一般形式的动理学方程, 并给出具有对称双曲形式的约化模型, 从而使得约化模型具有局部适定性。

Multiple Relational Ranking in Tensor: Theory, Algorithms and Applications

吴国宝²

Abstract: In this talk, I discuss multiple relational ranking problems arising from tensor data. Multi-Rank algorithms and its relevant mathematical results (convergence, higher-order Markov chains, transition probability tensors and perturbation bounds) are presented. Applications in data mining and information retrieval are given to demonstrate the performance and usefulness of the proposed algorithm.

¹李若, 北京大学. Email: rli@math.pku.edu.cn

²吴国宝, 香港浸会大学. Email: mng@math.hkbu.edu.hk

特邀大会报告

大数据分析技术图谱与研究举例

徐宗本³

Abstract: 大数据分析处理依赖特定的计算模式与全新的计算方法（称为大数据算法），设计创新的大数据计算模式与大数据算法是大数据的最核心技术，也是一个全新的领域。本报告引进大数据算法的谱系，并引进最优化理论与方法中的 ADMM (Alternating Direction Method of Multipliers) 作为大数据计算模式与算法设计的基本框架。我们说明：ADMM 非常适宜于实现“数据分解、变量分组、随机化”等大数据算法设计原理，并通过应用于大数据回归、超大规模线性方程组等问题展示 ADMM 方法的有效性。我们也说明：ADMM 能够解释作深度学习网络，从而 ADMM 理论与深度学习方法结合，能形成一类全新的“模型与数据”双驱动的大数据学习技术。该类技术能很好解决深度学习拓扑结构确定难的问题，也能很好解决 ADMM 难以用于模型族的问题。我们运用新技术学习 MRI 压缩感知成像取得了目前已知最好的效果，验证了新技术的可用性与高效性。

³徐宗本, 西安交通大学. Email: zbxu@mail.xjtu.edu.cn

Mixed Finite Element Methods based on Differential Complexes

陈龙⁴

Abstract: We shall present a systematically study of the mixed finite element methods based on differential complexes and the corresponding Helmholtz decomposition.

Firstly, we use the differential complexes to construct fast solvers for the saddle point systems arising from the mixed finite element methods. We discuss two type of fast solvers:

- Constraint optimization methods: Darcy equations, Stokes equations, and Kirchhoff plate bending problems.
- Preconditioners based on approximated block factorization: the Hodge Laplacian, Maxwell and the linear elasticity equations

Secondly, we analyze adaptive finite element methods based on the differential complexes. In particular, we discuss

- A posterior error estimates for symmetric conforming mixed finite elements for linear elasticity
- Convergence of adaptive mixed finite element methods for the Hodge Laplacian equations

Finally, we utilize the Helmholtz decomposition to decouple the mixed formulation of high order elliptic equations into combination of Poisson-type and Stokes-type equations. Examples include but not limit to: the biharmonic equation, the tri-harmonic equation, the fourth order curl equation, HHJ mixed method for plate problem, and Reissner-Mindlin plate model etc.

Fully Nonlinear Second Order PDEs and Their Numerical Solutions

凤小兵⁵

Abstract: In this talk I will present some latest advances on developing efficient numerical methods for fully nonlinear second (and first) order PDEs such as the Monge-Ampere type equations and Hamilton-Jacobi-Bellman equations. The focus of the talk will be on discussing various approaches/methods/ideas and their pros and cons for constructing such methods which can reliably approximate viscosity solutions of those fully nonlinear PDEs. Numerical experiments and applications as well as open problems in numerical fully nonlinear PDEs will also be presented.

⁴陈龙, University of California at Irvine, Beijing Institute for Scientific and Engineering Computing. Email: chenlong@math.uci.edu

⁵凤小兵, 美国田纳西大学, 西北工业大学. Email: xfeng@math.utk.edu

Alternating direction methods with multipliers for optimization problems involving nonconvex functions

韩德仁⁶

Abstract: Alternating direction method of multiplier (ADMM) is among the most efficient methods for solving the minimization problems where the objective function is the sum of several separable functions and the constraint is linear. While there are a lot of variants and convergence analysis for the convex case, the convergence for the problems involving nonconvex functions is in its infancy. In this talk, we introduce some advances for ADMM along this line. We split the results into two classes: the first class is based on the Kurdyka-Lojasiewicz inequality, and the second class is for some special models. Under some further conditions on the problem's data, we also analyze their rates of convergence.

千万核可扩展全隐式求解器：算法、实现与应用

杨超⁷

Abstract: 隐式求解器在大规模科学与工程计算应用领域具有广泛用途，是提高不少具体应用问题实际模拟效率的推进器。近年来，高性能计算机硬件体系结构呈现向异构、众核发展的趋势，隐式求解器的设计遇到了前所未有的挑战。我们的研究团队历经近十年努力，在面向当代甚至未来高性能计算机体系结构的隐式求解器设计方面取得进展，相关工作于2016年获得由美国计算机学会颁发的“戈登·贝尔”奖（ACM Gordon Bell Prize）。本次报告中，我将简单介绍我对“戈登·贝尔”奖的一些个人理解，并详细介绍我们2016年度的获奖工作。

Weak Galerkin Finite Element Scheme and Its Applications

张然⁸

Abstract: The weak Galerkin (WG) finite element method is a newly developed and efficient numerical technique for solving partial differential equations (PDEs). It was first introduced and analyzed for second order elliptic equations and further applied to several other model equations, such as the Brinkman equations, the eigenvalue problem of PDEs to demonstrate its power and efficiency as an emerging new numerical method. This talk introduces some progress on the WG scheme, which includes the applications on Brinkman problems, etc.

⁶韩德仁, 南京师范大学. Email: handeren@njnu.edu.cn

⁷杨超, 中国科学院软件研究所. Email: yangchao@iscas.ac.cn

⁸张然, 吉林大学. Email: zhangran@jlu.edu.cn

大规模矩阵近似的随机算法

张志华⁹

Abstract: 许多机器学习问题可以被关联为矩阵分解问题，因此求解大规模的矩阵分解问题是机器学习一个非常具有挑战性的课题。这个报告将关注于求解问题的随机算法，它是理论计算机科学、数值线性代数和应用统计分析的一个交叉领域。具体地，报告讨论矩阵乘积、SVD 和 CUR 分解等经典问题的随机近似算法。同时，将讨论矩阵近似技术在二阶优化算法的应用，包含子采样牛顿方法、概略牛顿方法以及非精确牛顿方法等。

三维不可压磁流体方程组的并行计算方法

郑伟英¹⁰

Abstract: 三维不可压磁流体 (MHD) 方程组描述带电流体在强磁场作用下的动力学行为，在磁约束聚变装置实验包层的数值模拟等领域有重要应用，流体的高 Hartmann 数给三维数值模拟带来很大挑战。本报告将讨论三方面的内容：(1) MHD 方程组的守恒型有限元方法，使得离散速度和磁场同时满足无散度约束条件；(2) 离散 MHD 方程组的健壮求解方法和工程 Benchmark 算例的并行计算；(3) 稳态 MHD 方程组的预处理技术和健壮求解方法。

⁹张志华, 北京大学. Email: zhzhang@math.pku.edu.cn

¹⁰郑伟英, 中科院数学与系统研究院. Email: zwy@lsec.cc.ac.cn

分会场报告 1

S02-1 非线性色散方程的数值方法

An efficient time-splitting compact finite difference method for nonlinear Schrodinger-type equations

王汉权¹¹

Abstract: Nonlinear Schrodinger-type equations are one of the most important models appeared in quantum physics, Bose-Einstein condensation, laser physics, and so on. We propose an efficient time-splitting compact finite difference method for nonlinear Schrodinger-type equations. In the first part of our talk, we propose an efficient time-splitting compact finite difference method for the Gross-Pitaevskii equation (GPE), we solve the GPE in time with time-splitting technique and in space by the compact finite difference method. To find the numerical solution of the resulting discretized system in one-dimension (1D), two-dimensions (2D) and three-dimensions (3D), we apply the fast discrete Sine transform in 1D, 2D and 3D respectively and get an efficient solver for the discretized system in 1D, 2D and 3D, respectively. Our numerical algorithm at every time step does not need linear-algebraic equations-solver, whose computation cost will be much higher when the spatial dimension increases. The method also has the merit that it is unconditionally stable and conservative. Moreover the method can achieve spectral-like accuracy in space when high-order compact finite difference method is applied. Extensive numerical tests for the GPE in 1D, 2D and 3D are presented to demonstrate the power and accuracy of the proposed numerical method. In the second part of our talk, we apply the time-splitting compact finite difference method into solving the nonlocal Gross-Pitaevskii equation (NGPE), which describes the dynamics of Bose-Einstein condensates (BEC) with dipole-dipole interaction at extremely low temperature. We present numerical examples in three dimensions to demonstrate the power of the proposed numerical method and discuss some physics of dipolar BEC.

¹¹王汉权, 云南财经大学. Email: wang_hanquan@hotmail.com

A uniformly accurate multiscale time integrator pseudospectral method for the nonlinear Dirac equation in the nonrelativistic limit regime

王燕¹²

Abstract: This talk is devoted to a multiscale time integrator Fourier pseudospectral (MTI-FP) method for the nonlinear Dirac equation (NLDE) with a dimensionless parameter which is inversely proportional to the speed of light. We first propose the MTI-FP method based on adopting a proper multiscale decomposition of the solution to the NLDE and applying the exponential wave integrator with appropriate numerical quadratures. Then, two independent error estimates are rigorously established for the proposed method, suggesting that the MTI-FP method converges uniformly and optimally in space with exponential convergence rate, and uniformly in time with linear convergence rate. At last, numerical results are reported to demonstrate that our error estimates are optimal and sharp.

Error bounds of finite difference time domain (FDTD) methods for the Dirac-Klein-Gordon equations

易雯帆¹³

Abstract: We propose and analyze finite difference methods for solving the coupled Dirac-Klein-Gordon (DKG) system. Due to the nonlinear coupling between the complex Dirac ‘wavefunction’ and the real Klein-Gordon field, it is a great challenges to design and analyze numerical methods for DKG. To overcome the difficulty induced by the nonlinearity, four implicit/semi-implicit/explicit finite difference time domain (FDTD) methods have been introduced, which are time symmetric or time reversible. Rigorous error estimates are established, and numerical results are reported to support our conclusion. The error analysis relies on the energy method, the special nonlinear coupling structure in DKG and the mathematical induction. Our approach is valid in one, two and three dimensions.

¹²王燕, 北京计算科学研究中心. Email: WANGY@NXU.EDU.CN

¹³易雯帆, 北京计算科学研究中心. Email: wfyi@csrc.ac.cn

Error estimates of finite difference method for Zakharov system in the subsonic limit

蔡勇勇¹⁴

Abstract: We rigorously analyze the error estimates of the conservative finite difference method (CNFD) for the Zakharov system (ZS) with a dimensionless parameter $\varepsilon \in (0, 1]$, which is inversely proportional to the ion acoustic speed. When $\varepsilon \rightarrow 0^+$, the ZS collapses to the standard nonlinear Schroedinger equation (NLS). In the subsonic limit i.e. $\varepsilon \rightarrow 0^+$, there exist highly oscillatory initial layers in the solution. The initial layers propagate with $O(\varepsilon)$ wavelength in time, $O(1)$ and $O(\varepsilon^2)$ amplitudes, for the ill-prepared initial data and well-prepared initial data, respectively. This oscillatory behavior brings significant difficulties in analyzing the errors of numerical methods for solving the Zakharov system. In this work, we show the CNFD possess the error bounds $h^2/\varepsilon + \tau^2/\varepsilon^3$ in the energy norm for the ill-prepared initial data, where h is mesh size and τ is time step. For the well-prepared initial data, the CNFD is uniformly convergent for $\varepsilon \in (0, 1]$, with second order accuracy in space and $O(\tau^{4/3})$ accuracy in time. This is a joint work with Yongjun Yuan.

Unconditional convergence of an alternating direction implicit finite difference scheme for the nonlinear Schrodinger equation in two dimensions

王廷春¹⁵

Abstract: This talk is concerned with the time-step condition of an alternating direction implicit finite difference scheme for solving the nonlinear Schrodinger equation in two dimensions. Besides the standard energy method, we introduce an induction argument and a ‘lifting’ technique as well as some useful inequalities to build the optimal maximum error estimate without any constraints on the time-step size. Numerical results are reported to support the theoretical analysis and show the effectiveness of the proposed scheme.

¹⁴蔡勇勇, 北京计算科学研究中心. Email: yongyong.cai@csrc.ac.cn

¹⁵王廷春, 南京信息工程大学. Email: wangtingchun@nuaa.edu.cn

Mathematical models and simulations for solid-state dewetting problems

蒋维¹⁶

Abstract: The Solid-state dewetting problem of thin films is a hot research topic which is attracting increasing attention from a lot of scientists. Studies on the solid-state dewetting problem involve in the multidisciplinary research, such as materials science, physics, applied mathematics, scientific computing and so on. Different from the traditional “liquid-wetting-solid” type problem, to some extent, the solid-state dewetting problem belongs to the “solid-wetting-solid” type problem. It includes two important research subjects, named as the surface diffusion flow and the moving contact line, and furthermore, the surface energy anisotropy plays important roles in the problem. In the talk, I will discuss several mathematical models which are used to simulate the solid-state dewetting problems, such as phase field model and sharp-interface model.

S06-1 偏微分方程反问题及其计算

Fourier method for the multi-frequency inverse source problems

郭玉坤¹⁷

Abstract: This talk is concerned with the inverse source problem of determining a source term in the Helmholtz equation from multi-frequency measurements. Based on the Fourier series expansion, we develop some novel non-iterative reconstruction schemes for solving the problem. The Fourier method is very fast and easy to implement, with robustness to measurement noise. Rigorous theoretical uniqueness and stability analysis will be provided. Numerical experiments will be presented to illustrate the effectiveness and efficiency of the proposed method in both two and three dimensions. This is a joint work with Xianchao Wang, Deyue Zhang and Hongyu Liu.

¹⁶蒋维, 武汉大学. Email: jiangwei1007@whu.edu.cn

¹⁷郭玉坤, 哈尔滨工业大学. Email: ykguo@hit.edu.cn

Increasing stability in the inverse source problem with attenuation and many frequencies

陆帅¹⁸

Abstract: We study the interior inverse source problem for the Helmholtz equation from boundary Cauchy data of multiple wave numbers. The main goal of this paper is to understand the dependence of increasing stability on the attenuation, both analytically and numerically. To implement it we use the Fourier transform with respect to the wave numbers, explicit bounds for analytic continuation, and observability bounds for the wave equation. In particular, by using Carleman estimates for the wave equation we trace the dependence of exact observability bounds on the constant damping. Numerical examples in 3 spatial dimension support the theoretical results. It is a joint work with Prof. Victor Isakov (Wichita State University).

Imaging of a local rough interface in a two-layered medium with possibly buried obstacles

杨家青¹⁹

Abstract: In this talk, I shall consider the inverse scattering associated with point sources from a local rough interface in a two-layered medium with some possible obstacles buried in the lower half-space. A uniqueness result is first proved for the inverse problem of recovering the local interface, the wavenumber and buried obstacles from the near-field data in the upper half-space. Then a novel version of the linear sampling method is developed to reconstruct the local rough interface based on such the data. Finally, the efficiency of the method is tested via several numerical simulations. This is a joint work with Prof. Bo Zhang (CAS) and Dr. Jianliang Li (CUST).

Near-field imaging of an inhomogeneous cavity with the factorization method

曲凤龙²⁰

Abstract: In this talk, I will introduce the inverse scattering of time-harmonic waves by an inhomogeneous cavity. We prove that the factorization method can be applied to recover the interior part of the inhomogeneous cavity from the near-field data measured inside the cavity. Finally, numerical examples are provided to illustrate the inversion algorithm.

¹⁸陆帅, 复旦大学数学科学学院. Email: slu@fudan.edu.cn

¹⁹杨家青, 西安交通大学. Email: jiaq.yang@xjtu.edu.cn

²⁰曲凤龙, 烟台大学.

Solvability of interior transmission problem for the diffusion equation and its applications

王海兵²¹

Abstract: Consider the interior transmission problem arising in inverse boundary value problems for the diffusion equation with discontinuous diffusion coefficients. We prove its unique solvability using the method of Green function. The key point is to construct the Green function for the interior transmission problem. We complete this procedure in the following way. First, we construct a local parametrix for the interior transmission problem near the boundary in the Laplace domain, by using the theory of pseudo-differential operators with a large parameter. Second, by carefully analyzing the analyticity of the Green function in the Laplace domain and estimating it there, a local parametrix for the original parabolic interior transmission problem is obtained via the inverse Laplace transform. Finally, using a partition of unity, we patch all the local parametrices and the fundamental solution of the diffusion operators to have a parametrix for the parabolic interior transmission problem, and then compensate it to get the Green function. Based on this solvability, we develop a sampling method for an inverse boundary value problem for the diffusion equation. This is a joint work with Prof. Gen Nakamura from Hokkaido University.

S07-1 流体力学方程的数学理论和数值方法

Compressible Euler equations and related problems

黄飞敏²²

Abstract: In this talk, I will present recent progress on the existence and uniqueness of entropy solutions of compressible Euler equations and related system, and introduce some open problems.

²¹王海兵, 东南大学. Email: hbwang@seu.edu.cn

²²黄飞敏, 中国科学院数学与系统科学研究院.

Direct Discontinuous Galerkin Method with Interface Correction

刘铁钢²³

Abstract: We prove that the original direct discontinuous Galerkin (DDG) method is not adjoint consistent. This leads to that the optimal order of accuracy cannot be reached when applied to adjoint-based optimization or mesh refinement. To fix this defect, an interface correction technique is proposed and leads to development of the direct discontinuous Galerkin method with interface correction (DDG(IC)). Theoretical analysis shows the extra interface correction term in DDG(IC) method plays a key role in both preserving the adjoint consistency and obtaining the optimal order of accuracy to the target functional computation. The performance of both DDG method and DDG(IC) method is carefully investigated and evaluated through typical test cases. Numerical experiments show that the DDG(IC) method can achieve the optimal order of accuracy with respect to the error in the computed target functional, which clearly indicates its superior potential compared to the original DDG method in the development and implementation of adjoint-based adaptation for simulating compressible flows.

A simple and efficient WENO method for hyperbolic conservation laws

邱建贤²⁴

Abstract: In this presentation, we present a simple high order weighted essentially non-oscillatory (WENO) schemes to solve hyperbolic conservation laws. The main advantages of these schemes presented in the paper are their compactness, robustness and could maintain good convergence property for solving steady state problems. Comparing with the classical WENO schemes by G.-S. Jiang and C.-W. Shu, J. Comput. Phys., 126 (1996), 202-228, there are two major advantages of the new WENO schemes. The first, the associated optimal linear weights are independent on topological structure of meshes, can be any positive numbers with only requirement that their summation equals to one, and the second is that the new scheme is more compact and efficient than the scheme by Jiang and Shu. Extensive numerical results are provided to illustrate the good performance of these new WENO schemes.

²³ 刘铁钢, 北京航空航天大学数学与系统科学学院. Email: liutg@buaa.edu.cn

²⁴ 邱建贤, 厦门大学数学科学学院. Email: jxqiu@xmu.edu.cn

Globally hyperbolic moment model of arbitrary order for special relativistic Boltzmann equation

汤华中²⁵

Abstract: We first extend the model reduction method by the operator projection to the 1D special relativistic Boltzmann equation. The derivation of arbitrary order globally hyperbolic moment system is built on our careful study of two families of the complicate Grad type orthogonal polynomials depending on a parameter. We derive their recurrence relations, calculate their derivatives with respect to the independent variable and parameter respectively, and study their zeros and coefficient matrices in the recurrence formulas. Some properties of the moment system are also proved. They include the eigenvalues and their bound as well as eigenvectors, hyperbolicity, characteristic fields, linear stability, and Lorentz covariance. A semi-implicit numerical scheme is presented to solve a Cauchy problem of our hyperbolic moment system in order to verify the convergence behavior of the moment method. The results show that the solutions of our hyperbolic moment system converge to the solution of the special relativistic Boltzmann equation as the order of the hyperbolic moment system increases. Now we are also deriving the globally hyperbolic moment model of arbitrary order for the 3D special relativistic Boltzmann eq. Moreover, it is interesting to develop robust, high order accurate numerical schemes for the moment system, find other basis for the derivation of moment system with some good property, e.g. non-negativity, and investigate the relativistic effects by using the moment system.

S08-1 无界域数学物理方程的数值方法及其应用

Effective boundary conditions for MD simulations

杨志坚²⁶

Abstract: This talk presents an absorbing boundary condition for molecular dynamics simulations of materials defects. The purpose of the boundary condition is to eliminates spurious reflections of phonons at the boundary and minimize the finite size effect. In contrast to other existing methods, our emphasis is placed on the ease of implementation. In particular, we propose a method for which the implementation can be done within existing molecular dynamics code, and it is insensitive to lattice structure, the geometry and space dimension of the computational domain. To demonstrate the effectiveness, the results from two test problems are presented.

²⁵汤华中, 北京大学数学科学学院、湘潭大学数学与计算科学学院. Email: hztang@math.pku.edu.cn

²⁶杨志坚, 武汉大学数学与统计学院. Email: zjyang.math@whu.edu.cn

HDG methods for the Maxwell equations

陈黄鑫²⁷

Abstract: In this talk we will first introduce a new HDG method for the steady state Maxwell equations based on a mixed curl-curl formulation. We use a non-trivial subspace of polynomials of degree $k+1$ to approximate the numerical tangential trace of the electric field and polynomials of degree $k+1$ to approximate the numerical trace of the Lagrange multiplier on the faces. If we assume the dual operator of the Maxwell equation has adequate regularity, we show that the order of convergence of L2-error for the electric field is $k+2$. From the point of view of degrees of freedom of the globally coupled unknown: numerical trace, this HDG method achieves super-convergence for the electric field without post-processing. In particular, the convergence rate of the electric field is independent of the Lagrange multiplier when the HDG scheme is based on simplicial mesh. When we consider the Maxwell equations with low regularity of electric field, another HDG method and its optimal convergence rate will be shown, and the corresponding adaptive HDG method will be discussed.

并行波源转移区域分裂算法

崔涛²⁸

Abstract: 我们使用谱元法离散时谐弹性波方程, 设计了并行波源转移区域分裂算法, 将其作为 GMRES 迭代算法的预条件子去求解离散问题。数值算例表明波源转移区域分裂算法可以作为常波数或变波数时谐弹性波散射问题的有效预条件子。对于常波数问题, 当采用适当高阶谱元格式降低离散误差时, 以波源转移区域分裂算法作为预条件子的 GMRES 迭代算法只需要非常少的迭代步数即可收敛。

Computational Issues on Kohn-Sham Equation

胡光辉²⁹

Abstract: In this talk, we will introduce our work on the adaptive finite element solutions of Kohn-Sham density functional theory, which is one of the most successful models in the electronic structure calculations. The challenges on designing quality numerical methods will be briefly summarized, and our methods on resolving those challenges follow. Numerical results show the effectiveness of our method.

²⁷陈黄鑫, 厦门大学数学科学学院. Email: chx@xmu.edu.cn

²⁸崔涛, 中国科学院数学与系统科学研究院. Email: tcui@lsec.cc.ac.cn

²⁹胡光辉, 澳门大学数学系. Email: garyhu@umac.mo

Artificial boundary conditions of nonlocal models on unbounded domains

张继伟³⁰

Abstract: The numerical solutions of nonlocal models such as nonlocal heat and wave equations on unbounded domains are considered. Differing from local models, the nonlocal effect makes the design of absorbing boundary conditions (ABCs) more difficulty since it breaks up the symmetry of the operator and requires an artificial layer to limit the bounded computational domain of interest. In this talk, we will report the recent progress on this topic. These works are jointed with Prof. Qiang Du, Prof. Houde Han and Prof. Chunxiong Zheng and so on.

S11-1 最优化专题

三个算子的交替方向类算法 (ADMM) 进展

何炳生³¹

Abstract: 数据科学中的不少问题可以归结为（或松弛成）一个凸优化问题. 乘子交替方向法 (ADMM) 是最优化提供给数据科学的重要方法. 交替方向法处理两个可分离算子线性约束凸优化问题已经比较成熟, 直接推广处理三个算子的问题却不能保证收敛, 除非外加一些难于验证的条件或者不太切合实际的假设. 报告回顾总结我们近 10 年来提出的处理三个算子的 ADMM 类方法, 它们共同特点是不对问题本身有任何额外的要求, 也不对参数选取做什么限制, 而是只对原来不能保证收敛的方法稍做改动, 就能保证算法收敛. 这些三个算子的方法都能推广到处理多个算子的问题. 报告同时也提出一些 ADMM 类方法中有意义而尚未解决的问题.

CMIP 混合整数规划求解器进展

戴戡虹³²

Abstract: Mixed integer linear program (MIP) has wide applications in many areas, including electrical power, energy, finance, work force management, transportation, etc. In this talk, we will present the software framework for MIP and our developing solver CMIP. The main ingredients of the solver will be presented, including the presolver, branch strategies, node selection strategies, cutting planes and primal heuristics. Furthermore, we will give a computational study to evaluate the performances impact of each ingredient in CMIP.

³⁰张继伟, 北京计算科学研究中心. Email: jwzhang@csrc.ac.cn

³¹何炳生, 南方科技大学/南京大学. Email: hehma@nju.edu.cn

³²戴戡虹, 中国科学院数学与系统科学研究院. Email: dyh@lsec.cc.ac.cn

复张量特征值计算

倪谷炎³³

Abstract: This talk introduces the computation of eigenpairs of high-order complex tensors, which is closely related to the best complex rank-one approximation of a tensor and quantum entanglement. It is also an optimization problem of real-valued functions with complex variables. We study the spherical optimization problem with complex variables including the first-order and the second-order Taylor polynomials, optimization conditions and convex functions of real-valued functions with complex variables. We propose an algorithm and show that it is guaranteed to approximate an eigenpair of a complex tensor. Moreover, if the number of eigenpair is finite, then the algorithm is convergent to an eigenpair. Numerical examples are presented to demonstrate the effectiveness of the proposed method in finding eigenpairs.

Structured Tensor and Complementarity Problem

宋义生³⁴

Abstract: This report deals with the class of Q-tensors, that is, a Q-tensor is a real tensor A such that the tensor complementarity problem (q, A) has a solution for each vector $q \in \mathbb{R}^n$. Several subclasses of Q-tensors are given: P-tensors, R-tensors, strictly semi-positive tensors and semi-positive R0-tensors. We prove that a nonnegative tensor is a Q-tensor if and only if all of its principal diagonal entries are positive, and so the equivalence of Q-tensor, R-tensors, strictly semi-positive tensors is showed if they are nonnegative tensors. We also show that a tensor is a R0-tensor if and only if the tensor complementarity problem $(0, A)$ has nonon zero vector solution, and a tensor is a R-tensor if and only if it is a R0-tensor and the tensor complementarity problem (e, A) has nonon-zero vector solution.

³³倪谷炎, 国防科技大学. Email: guyan-ni@163.com

³⁴宋义生, 河南师范大学. Email: songyisheng@htu.cn

On Glowinski's Open Question of Alternating Direction Method of Multipliers

陶敏³⁵

Abstract: The alternating direction method of multipliers (ADMM) was proposed by Glowinski and Marrocco in 1975; and it has been widely used in a broad spectrum of areas, especially in some sparsity-driven application domains. In 1982, Fortin and Glowinski suggested to enlarge the range of the step size for updating the dual variable in ADMM from 1 to $(0, \frac{1+\sqrt{5}}{2})$; and this strategy immediately accelerates the convergence of ADMM for most of its applications. Meanwhile, Glowinski raised the question of whether or not the range can be further enlarged to $(0, 2)$; this question remains open with nearly no progress in the past decades. In this paper, we answer this question affirmatively for the case where both the functions in the objective are quadratic. Glowinski's open question is thus partially answered. We further establish the global linear convergence of the ADMM with the step size range $(0, 2)$ for the quadratic programming case under a condition that turns out to be tight.

S13-1 生命科学中的计算数学

基于三层数据融合的药物-疾病关系预测模型

刘娟³⁶

Abstract: 药物-疾病关系的发现有助于老药新用和老病新治。我们提出了一种异质数据分层融合的方法，并基于相似的药物-疾病关系对具有相似的治疗模式这一假设，将药物-疾病关系预测问题转化为最优图分割问题。为此，我们构建了以药物-疾病关系对为节点的加权图，并提出了半监督的图分割方法。

³⁵陶敏, 南京大学. Email: taom@nju.edu.cn

³⁶刘娟, 武汉大学.

离子通道模型与有限元模拟

卢本卓³⁷

Abstract: 基于离子通道蛋白结构的连续模型能够连接微观到宏观的尺度, 直接观测到通道内离子电流的宏观动态过程。本报告介绍我们发展的几个模型及 3 维有限元模拟方法。在传统的 Poisson-Nernst-Planck 模型上, 可进一步考虑离子的尺寸效应、变介电系数、溶剂化能等改进模型, 研究分子结构、几何形状、静电相互作用、及离子特性等对离子通透性的影响。计算上发展了有限元计算方法、分子网格生成及优化技术、在线计算平台等。计算结果表明, 通常对于较大的孔道或纳米管, PNP 就能很好的描述电压-电流特性、整流效应等导电性质; 狭窄通道如钾离子通道, 我们的新模型也能刻画出通道内钾离子的选择性结合以及高于钠离子的通透性; 离子尺寸修改模型能合理地反应出蛋白表面和通道内的离子浓度的饱和现象。这些方法和软件也可用于若干其它领域, 如酶分子的电扩散反应过程、纳米孔基因测序、半导体器件模拟等。

The phenotypic equilibrium of cancer cells: From average-level stability to path-wise convergence

牛原玲³⁸

Abstract: The phenotypic equilibrium, i.e. heterogeneous population of cancer cells tending to a fixed equilibrium of phenotypic proportions, has received much attention in cancer biology very recently. In the previous literature, some theoretical models were used to predict the experimental phenomena of the phenotypic equilibrium, which were often explained by different concepts of stabilities of the models. Here we present a stochastic multi-phenotype branching model by integrating conventional cellular hierarchy with phenotypic plasticity mechanisms of cancer cells. Based on our model, it is shown that: (i) our model can serve as a framework to unify the previous models for the phenotypic equilibrium, and then harmonizes the different kinds of average-level stabilities proposed in these models; and (ii) path-wise convergence of our model provides a deeper understanding to the phenotypic equilibrium from stochastic point of view. That is, the emergence of the phenotypic equilibrium is rooted in the stochastic nature of (almost) every sample path, the average-level stability just follows from it by averaging stochastic samples.

³⁷ 卢本卓, 中国科学院.

³⁸ 牛原玲, 中南大学.

Systematic development of stable numerical methods for nonequilibrium dissipative systems with applications to life science

王奇³⁹

Abstract: Life is a process consisting of energy generation and energy dissipation. Any equation systems, devised to describe a live system, must possess the two features. Idealistically, when the energy generating mechanism is shut off, the system should be dissipative. I will discuss a systematic approach to developing energy stable numerical methods for a general nonequilibrium dissipative hydrodynamic system. When coupled with the energy generating mechanism, the coupled system can be used to describe a live system or active matter system. For the coupled system, the numerical methods are required to respect the energy dissipation rate, which may not be dissipative at all. Numerical examples for cell migration and oscillation will be presented to illustrate the usefulness of the new methods.

Multiensemble Markov models of molecular thermodynamics and kinetics

吴昊⁴⁰

Abstract: Molecular dynamics (MD) simulations have become important tools in the investigation of biomolecular processes. However, important biological processes with long time scales, such as protein conformational transitions and protein–ligand dissociation, are still out of reach for unbiased MD simulation. Two typical strategies are (i) conducting large ensembles of short simulations and estimating the long-term kinetics with a Markov state model, and (ii) speeding up rare events by bias potentials or higher temperatures and estimating the unbiased thermodynamics with reweighting estimators. In this talk, I will introduce the transition-based reweighting analysis method (TRAM), a statistically optimal approach that combines the best of both worlds and estimates a multiensemble Markov model (MEMM) with full thermodynamic and kinetic information at all simulated ensembles.

³⁹王奇, 北京计算科学研究中心、南卡大学.

⁴⁰吴昊, 柏林自由大学.

T01-1 微分方程数值计算及应用

线性微分系统重构的数值算法

李崇君⁴¹

Abstract: 在一些实际工程问题中, 需要用线性微分系统进行数学建模, 例如在计算机辅助设计和制造中, 利用线性微分系统进行曲线曲面表示, 将更容易表达曲线曲面具有的动力学性质。在本报告中, 我们将介绍基于离散数据点的线性微分系统重构的数值算法, 包括重构常系数和变系数的线性微分系统。这些算法可用于曲线曲面的拟合, 即采用微分系统的解曲线和解曲面去逼近离散采样的数据点。通过一些数值算例, 显示出重构算法具有很好的逼近精度。

Kernel-based Approximation Methods for Partial Differential Equations: Deterministic or Stochastic Problems?

Qi Ye⁴²

Abstract: In this talk, we present the kernel-based approximation methods to solve the partial differential equations by the Gaussian process regressions defined on the kernel-based probability spaces induced from the positive definite kernels. We focus on the kernel-based regression solutions of the multiple Poisson equations. Using the kernel-based probability measures, we show many properties of the kernel-based regression solutions including approximate formulas, convergence, acceptable errors, and optimal initialization. Generally, we combine the knowledge and techniques of numerical analysis, regression analysis, and stochastic analysis to renew the theory of kernel-based approximation methods.

Recent development in numerical simulations of molecular beam epitaxial equations

乔中华⁴³

Abstract: Recently, the molecular beam epitaxy (MBE) has become an important technique for the growth of thin films. By using the MBE technique, it is possible to grow high-quality crystalline materials and form structures with high precision in the vertical direction. There has been a large amount of research interest in the dynamics of the MBE growth. A sufficiently long integration time is necessary in order to detect the epitaxy growth behaviors and to reach the physical scaling regime. To carry out numerical simulations with large time and large computational domain, highly stable and accurate numerical schemes are required. In this talk, our recent works on numerical simulations of these MBE models will be presented.

⁴¹ 李崇君, 大连理工大学数学科学学院. Email: chongjun@dlut.edu.cn

⁴² 叶颀, 华南师范大学. Email: yeqi@m.scnu.edu.cn

⁴³ 乔中华, 香港理工大学. Email: zqiao@polyu.edu.hk

Unconditional and optimal H2-error estimates of two linear and conservative finite difference schemes for the Klein-Gordon-Schrodinger equation in high dimensions

王廷春, 赵晓飞, 蒋佳平⁴⁴

Abstract: The focus of this paper is on the optimal error bounds of two finite difference schemes for solving the d-dimensional ($d=2,3$) nonlinear Klein-Gordon-Schrodinger (KGS) equations. The proposed finite difference schemes not only conserve the mass and energy in the discrete level but also are efficient in practical computation because only two linear systems need to be solved at each time step. Besides the standard energy method, an induction argument as well as a ‘lifting’ technique are introduced to establish rigorously the optimal H2-error estimates without any restrictions on the grid ratios, while the previous works either are not rigorous enough or often require certain restriction on the grid ratios. The convergence rates of the proposed schemes are proved to be at $O(h^2 + \tau^2)$ with mesh-size h and time step τ in the discrete H2-norm. The analysis method can be directly extended to other linear finite difference schemes for solving the KGS equations in high dimensions. Numerical results are reported to confirm the theoretical analysis for the proposed finite difference schemes.

A mass conserving lattice Boltzmann scheme for diffuse interface model with different equation of states

杨旭光, 乔中华⁴⁵

Abstract: In this work, a realistic diffuse interface model with different equation of states (EOS) for two-phase fluid systems are numerically studied by the lattice Boltzmann (LB) method. Based on the gradient theory of thermodynamics and variational calculus, a generalized chemical equilibrium equation is obtained with extremely strong nonlinear source term. Through adding a time-derivative term, the steady-state equation is converted to a time-dependent parabolic partial differential equation (PDE). In addition, a Lagrange multiplier is introduced to enforce mass conservation. And then, a mass conserving LB scheme is proposed to solve this transient system. The Lagrange multiplier is defined based on the mesoscopic character of the proposed LB scheme. Furthermore, using the multi-scale Chapman-Enskog analysis, the time-dependent parabolic PDE can be recovered with second order accuracy from the proposed LB scheme. Finally, the three-dimensional numerical simulations of realistic hydrocarbon components, such as isobutane and propane, are implemented to illustrate the theory. The numerical results reach a good agreement with laboratory data when the width of the two-phase interface is considered.

⁴⁴王廷春, 南京信息工程大学. Email: wangtingchun@nuaa.edu.cn

⁴⁵杨旭光, 湖南第一师范学院. Email: xuguang1988@163.com

High-accuracy algorithms for one dimensional singular interface problems

YaNan Jia(贾亚男), ZhiYue Zhang(张志跃)⁴⁶

Abstract: This paper presents a numerical method for one dimensional interface problems with a singular variable coefficient that has a finite jump across the interface. The key of the idea is that the interface problem can be fully decoupled as two-point boundary value problems with undetermined parameters and then we just need to solve the two decoupled problems. Some numerical examples are presented to show the high-accuracy solution and the high-accuracy gradient in the entire domain with lower computation cost.

T03-1 优化、控制及反问题

Regularization Parameter Selection for Total Variation Based Image Restoration

文有为⁴⁷

Abstract: The problem of image restoration is ill-conditioned. A total variation based regularization method should be used in the image restoration process. It is a very important task to select a suitable regularization parameter. By adjusting regularization parameter, a compromise is achieved to suppress the noise and preserve the nature of the original image. The appropriate compromise highly depends on the choice of the regularization parameter. Usually, regularization parameter is determined manually by trial-and-error method, the generalized cross validation (GCV) method, the L-curve method, the discrepancy principle, etc. In this talk, we will introduce some methods how to choose the regularization parameter for total variation based image restoration.

⁴⁶贾亚男, 南京师范大学. Email: jiayanangd@163.com

⁴⁷文有为, 湖南师范大学. Email: wenyowei@gmail.com

A new TV-Stokes model for image deblurring and denoising with fast algorithms

Zhi-Gang Jia and Musheng Wei⁴⁸

Abstract: The famous TV-Stokes models, which improve the restored images comfortable, have been very successful in image denoising. In this paper, we propose a new TV-Stokes model for image deblurring with a good geometry explanation. In the tangential field smoothing, the data fidelity term is chosen to measure the distance between the solution and the orthogonal projection of the tangential field of the observation image onto the range of the conjugate of the blurry operator, while the total variation of the solution is chosen as the regularization term. In the image reconstruction, we compute the smoothing part of the image from the smoothed tangential field for the first step, and use an anisotropic TV model to obtain the “texture” part of the deblurred image. The solvability properties for the minimization problems in two steps are established, and fast algorithms are presented. Numerical experiments demonstrate that the new deblurring model can capture the details of images hidden in the blurry and noisy image, and the fast algorithms are efficient and robust.

A globally convergent method for computing fixed point of self-mapping on general nonconvex set

祝志川⁴⁹

Abstract: In this paper, to compute the fixed point of self-mapping on general nonconvex sets with both inequality and equality constraints, a feasible set swelling homotopy is constructed and the existence and global convergence of the smooth homotopy pathways is proved under some mild conditions. Compared with the previous results, the initial point is not needed to be a feasible interior point of the original feasible set, and can be chosen freely in a bounded ball region of the shifted feasible set. Some numerical examples are also given to show the feasibility and effectiveness of the homotopy method.

⁴⁸贾志刚, 数学与统计学院/江苏师范大学. Email: zhgjia@jsnu.edu.cn

⁴⁹祝志川, 吉林财经大学. Email: zhuzcnh@126.com

An efficient Peaceman-Rachford splitting method for constrained TGV-shearlet based MRI reconstruction

Tingting Wu, Wenxing Zhang, David Z. W. Wang, and Yuehong Sun⁵⁰

Abstract: In this paper, we propose a constrained total generalized variation and shearlet transform based model for magnetic resonance imaging reconstruction, which is usually more undemanding and practical to identify appropriate tradeoffs than its unconstrained counterpart. The proposed model can be facilely and efficiently solved by the strictly contractive PeacemanRachford splitting method, which generally outperforms some state-of-the-art algorithms when solving separable convex programming. Numerical simulations demonstrate that the sharp edges and grainy details in magnetic resonance images can be well reconstructed from the undersampling data.

Tikhonov Regularization and Randomized GSVD

Yimin Wei, Pengpeng Xie and Liping Zhang⁵¹

Abstract: The generalized singular value decomposition (GSVD) is one of the essential tools in numerical linear algebra. This paper proposes a regularization method, combining Tikhonov regularization in general form with the truncated GSVD. Then the randomized algorithms are adopted to implement the truncation process. This randomized GSVD for the regularization of the large-scale ill-posed problems can achieve good accuracy with less computational time and memory requirement than the classical regularization methods. Finally, we present the error analyses for the randomized algorithms. Some illustrative numerical examples are provided.

PET-MRI Joint Reconstruction by Joint Sparsity Based Tight Frame Regularization

Jae Kyu Choi, Chenglong Bao, Xiaoqun Zhang⁵²

Abstract: Recent technical advances lead to the coupling of PET and MRI scanners, enabling to acquire functional and anatomical data simultaneously. In this talk, we propose a wavelet tight frame based PET-MRI joint reconstruction model via the joint sparsity of tight frame coefficients. In addition, a non-convex balanced approach is adopted to take the different sparsity patterns of PET and MRI images into account. To solve the nonconvex and nonsmooth model, a proximal alternating minimization algorithm is proposed, and the global convergence is present based on Kurdyka-Lojasiewicz property.

⁵⁰ 武婷婷, 南京邮电大学. Email: wutt@njupt.edu.cn

⁵¹ 张理评, 浙江工业大学. Email: zhanglp@zjut.edu.cn

⁵² 崔宰珪, 上海交通大学. Email: jaycjk@sjtu.edu.cn

T06-1 有限元和边界元方法

High-Order Extended Finite Element Methods for Solving Interface ProblemsYuanming Xiao, Haijun Wu, Jinchao Xu, Fei Wang, Peiqi Huang⁵³

Abstract: Two different discontinuous Galerkin (DG) schemes on arbitrary order extended finite element (XFE) spaces are proposed for solving elliptic interface problems. Optimal error estimates in the piecewise H^1 -norm and in the L^2 -norm are rigorously proved for both schemes. In particular, we have devised a new parameter-friendly DG-XFEM method, which means that no “sufficiently large” parameters are needed to ensure the optimal convergence of the scheme. To prove the stability of bilinear forms, we derive non-standard trace and inverse inequalities for high-order polynomials on curved sub-elements divided by the interface. All the estimates are independent of the location of the interface relative to the meshes. Numerical examples are given to support the theoretical results.

Unconditional stability and error estimates of modified characteristics Finite Element Methods司智勇⁵⁴

Abstract: The paper is concerned with the unconditional stability and convergence of characteristics type methods for the time-dependent Navier–Stokes equations. We present optimal error estimates in L^2 and H^1 norms for a typical modified characteristics finite element method unconditionally, while all previous works require certain time-step restrictions. The analysis is based on an iterated characteristic time-discrete system, with which the error function is split into a temporal error and a spatial error. With a rigorous analysis to the characteristic time-discrete system, we prove that the difference between the numerical solution and the solution of the time-discrete system is τ -independent, where τ denotes the time stepsize. Thus numerical solution in $W^{1,\infty}$ is bounded and optimal error estimates can be obtained in a traditional way. Numerical results confirm our analysis and show clearly the unconditional stability and convergence of the modified characteristics finite element method for the time-dependent Navier–Stokes equations. The approach used in this paper can be easily extended to many other characteristics-based methods.

⁵³肖源明, 南京大学. Email: xym@nju.edu.cn⁵⁴司智勇, 河南理工大学. Email: sizhiyong@hpu.edu.cn

Mesh quality and more detailed error estimates of finite element method

Yunqing Huang, Liupeng Wang and Nianyu Yi⁵⁵

Abstract: In this talk, we show the role of mesh quality on the accuracy of linear finite element approximation. We derive a more detailed error estimate, which shows explicitly how the shape and size of elements, and symmetry structure of mesh effect on the error of numerical approximation. Two computable parameters G_e and G_v are given to depict the cell geometry property and symmetry structure of the mesh. In compare with the standard a priori error estimates, which only yield information on the asymptotic error behaviour in a global sense, our proposed error estimate considers the effect of local element geometry properties, and is thus more accurate. Under certain conditions, the traditional error estimates and superconvergence results can be derived from the proposed error estimate. Moreover, the estimators G_e and G_v are computable and thus can be used for predicting the variation of errors.

low order conforming mixed finite element methods for elasticity on simplicial grids

Yang Yan, Xie Xiaoping⁵⁶

Abstract: In this talk, we will present low order conforming mixed finite element methods with symmetric stress approximation for elasticity on simplicial grids in R^n ($n=2,3$). We use the piecewise $P_2 - P_1$ and $P_3 - P_2$ combinations to approximate the stress and displacement variabes in the two- and three- dimensional cases, respectively. We show t the inf-sup stability and derive optimal error estimates. Numerical results confirm the theoretical analysis.

Fast and stable evaluation of the exact absorbing boundary condition for the semi-discrete linear Schrodinger equation in unbounded domains

胡嘉顺⁵⁷

Abstract: This report is concerned with the numerical solution of the one-dimensional linear Schrodinger equation in unbounded domains. In order to compute the solution on the domain of physical interest, we apply the artificial boundary method to transform the unbounded problem into an initial boundary value problem. Then, the stability of the derived problem is proved, and fast algorithm is given to approximate the nonlocal boundary conditions. The novelty of this fast algorithm is that the stability of the approximate truncated semi-discrete problem is automatically maintained.

⁵⁵ 易年余, 湘潭大学. Email: yinianyu@xtu.edu.cn

⁵⁶ 杨艳, 西南石油大学. Email: 289607684@qq.com

⁵⁷ 胡嘉顺, 清华大学. Email: hjs16@mails.tsinghua.edu.cn

Analysis of Galerkin FEMs for mixed formulation of time-dependent Ginzburg-Landau equations under temporal gauge

Chengda Wu, Weiwei Sun⁵⁸

Abstract: Numerical solution of time-dependent Ginzburg–Landau (GL) equations under the temporal gauge (zero electric potential gauge) is a most popular tool in the study of vortex dynamics in superconductors. The paper focuses on the analysis of linearized Galerkin FEMs for a mixed formulation of the time dependent Ginzburg–Landau (GL) equations under the temporal gauge. We provide optimal error estimates in L^2 -norm for the order parameter ψ and the magnetic field σ unconditionally, although the accuracy of numerical magnetic potential A is one order lower than optimal one due to the degeneracy of magnetic potential equation. Since the states of superconductors are determined by the order parameter ψ (or the density of the superconducting electron pairs $|\psi|$), the accuracy of ψ is more important in the vortex simulation. Our analysis is based on a non-classical Ritz projection, which may reduce the pollution of inaccuracy of numerical magnetic potential in the analysis. Numerical experiments confirm our theoretical analysis.

A Cartesian grid nonconforming immersed finite element method for planar elasticity interface problems

Fangfang Qin, Jinru Chen, Zhilin Li, Mingchao Cai⁵⁹

Abstract: In this paper, a new nonconforming immersed finite element (IFE) method on triangular Cartesian meshes is developed for solving planar elasticity interface problems. The proposed IFE method possesses optimal approximation property for both compressible and nearly incompressible problems. Its degree of freedom is much less than those of existing finite element methods for the same problem. Moreover, the method is robust with respect to the shape of the interface and its location relative to the domain and the underlying mesh. Both theory and numerical experiments are presented to demonstrate the effectiveness of the new method. Theoretically, the unisolvent property and the consistency of the IFE space are proved. Experimentally, extensive numerical examples are given to show that the approximation orders in L^2 norm and semi- H^1 norm are optimal under various Lamé parameters settings and different interface geometry configurations

⁵⁸WU Chengda, City University of Hong Kong. Email: chengdawu2-c@my.cityu.edu.hk

⁵⁹秦芳芳, 南京师范大学. Email: qff890505@163.com

T09-1 分数阶方程

The finite difference method for Caputo-type parabolic equation with fractional Laplacian李常品⁶⁰

Abstract: In this talk, we present the finite difference method for Caputo-type parabolic equation with fractional Laplacian, where the time derivative is in the sense of Caputo with order in $(0, 1)$ and the spatial derivative in the fractional Laplacian. The stability, convergence, and error estimate are displayed. And illustrative examples are also provided which support the theoretical analysis.

分数阶双延迟纳米热传导模型和数值方法

纪翠翠（东南大学），戴伟忠（美国路易斯安娜科技大学），孙志忠（东南大学）⁶¹

Abstract: 纳米热传导具有许多有别于宏观尺度下的热传导的特征。获得纳米结构下的精确的温度分布是认识纳米器件热传导过程的关键。本工作提出了基于双延迟热传导方程的新的分数阶纳米热输运模型，证明了模型的适定性。给出了差分方法求解这一分数阶纳米热输运模型，并用能量方法证明了差分格式的无条件稳定性和收敛性。数值例子证实了理论结果。

Nonuniform L1 formula and discrete Gronwall inequality for time-fractional reaction-subdiffusion equationsHong-lin Liao⁶²

Abstract: Stability and convergence of the L1 formula on nonuniform grids are investigated for solving Caputo fractional reaction-subdiffusion equations. A discrete Gronwall-type inequality is developed for the nonuniform L1 formula by introducing a discrete convolution kernel of Riemann-Liouville fractional integral. To simplify the consistence analysis of nonuniform L1 formula, we bound the local truncation error by a discrete convolution form with the L1 coefficients, and consider a global convolution error with the discrete Riemann-Liouville integral kernel. With the help of discrete fractional Gronwall-type inequality and global consistence error analysis, a new L^2 -norm error estimate reflecting the regularity of solution is obtained for a simple discrete scheme on nonuniform time meshes. Numerical tests are provided to confirm the sharpness of error analysis.

⁶⁰李常品, 上海大学. Email: lcp@shu.edu.cn⁶¹孙志忠, 东南大学. Email: zzsun@seu.edu.cn⁶²廖洪林, 解放军陆军工程大学. Email: liao hl@csrc.ac.cn

Mapped Jacobi Spectral Methods for Singularly Perturbed Problems of Fractional Order

Sun Tao⁶³

Abstract: In this talk, we first investigate the mapped Jacobi polynomials and their properties of fractional integration and derivation, and find out that they belong to a kind of special Müntz-Legendre polynomials. The approximation of mapped Jacobi polynomials are studied afterwards. As applications, we propose mapped Jacobi spectral-Petrov-Galerkin and spectral-Galerkin methods for singularly perturbed Caputo FIVPs and Riesz FBVPs, which can derive diagonal or tri-diagonal and symmetric well conditioned stiffness matrices. Meanwhile, we use some examples to indicate the efficiency and high accuracy of the corresponding numerical schemes. This is a joint work with Dr. Liu Rui-qing and Prof. Wang Li-lian.

Energy Stable Numerical Schemes for Some Classical and Nonlocal Phase Field Models

李晓⁶⁴

Abstract: In this talk, we focus on the energy stable schemes for some phase field models. First, we present two nonlinear schemes for a Cahn-Hilliard-like equation with variable interfacial coefficient, modeling the microstructure of the macromolecular microsphere composite hydrogel, by using the convex splitting technique. Then, we consider the exponential time differencing (ETD) method for the epitaxial growth model without slope selection and establish the energy stability and error estimates of the proposed explicit ETD schemes. Next, in our newest work, we consider a class of nonlocal Cahn-Hilliard equations corresponding to an energy functional coming from the classical Ginzburg-Landau free energy with the Laplacian replaced by a well-defined nonlocal diffusion operator. The lack of the high order diffusion term becomes the main difficulty for the numerical analysis and the nonlocal term usually leads to expensive calculations. We propose the stabilized linear semi-implicit schemes with first and second order temporal accuracy by adding an artificial term and analyze the energy stability and error estimates. Numerical experiments are presented to make a comparison of the phase transition process with the corresponding local case.

⁶³ 孙涛, 上海立信会计金融学院. Email: stao_2004@126.com

⁶⁴ 李晓, 北京计算科学研究中心. Email: lixiao1228@163.com

Stability and convergence of a fully-discrete local discontinuous Galerkin method for multi-term time fractional diffusion equations

韦雷雷⁶⁵

Abstract: In this paper a fully discrete local discontinuous Galerkin method for a class of multi-term time fractional diffusion equations is proposed and analyzed. Using local discontinuous Galerkin method in spatial direction and classical $L1$ approximation in temporal direction, a fully-discrete scheme is established. By choosing the numerical flux carefully, we prove that the method is unconditionally stable and convergent with order $O(h^{k+1} + (\Delta t)^{2-\alpha})$, where $k, h, \Delta t$ are the degree of piecewise polynomial, the space and time step sizes, respectively. Numerical examples are carried out to illustrate the effectiveness of the numerical scheme.

分会场报告 2

S06-2 偏微分方程反问题及其计算

Carleman estimate and applications for piezoelectric equations

徐翔⁶⁶

Abstract: In this talk, Carleman estimate for piezoelectric equations in one dimension is established. Utilizing this estimate, a local Holder stability for an inverse source problem is obtained on determining a spatial component. Consequently, we show a uniqueness and Lipschitz stability result on an inverse coefficient problem in case of interior observation data. Moreover, the inverse source and coefficient problems are numerically solved via an iterative algorithm based upon regularization methods. Numerical examples are presented to validate the effectiveness of the proposed algorithms.

⁶⁵ 韦雷雷, 河南工业大学. Email: leileiwei@haut.edu.cn

⁶⁶ 徐翔, 浙江大学. Email: xxu@zju.edu.cn

Numerical solution of scattering and inverse scattering for rough surfaces

张磊 (HLJU)⁶⁷

Abstract: In this talk, we consider the acoustic scattering and inverse scattering problems by a kind of rough surface with tapered incidence. We derive the boundary integral equation and the validity of the integral equation formulation is proved. Numerical solution is needed in a finite interval, so existence and uniqueness of the solution for the truncated problem as well as the convergence of the truncation method are established. Then a numerical inversion method to identify the rough surfaces from the phaseless measurements of the scattered field at a fixed frequency is developed. Numerical examples are presented to show the validity and efficiency of the proposed method.

Inverse scattering problem from phaseless far-field data

张海文⁶⁸

Abstract: It is well known that the modulus of the far-field pattern (or phaseless far-field pattern) is invariant under translations of the scattering obstacle if only one plane wave is used as the incident field, so the shape but not the location of the obstacle can be recovered from the phaseless far-field data. In this talk, it is proved that the translation invariance property of the phaseless far-field pattern can be broken if superpositions of two plane waves are used as the incident fields. Based on this, a direct imaging method is then developed to recover both the location and the shape of the obstacle simultaneously from multi-frequency phaseless far-field data. Numerical examples are also carried out to illustrate the validity of the approach and the effectiveness of the inversion algorithm.

⁶⁷张磊 (HLJU), 黑龙江大学.

⁶⁸张海文, 中国科学院数学与系统科学研究院. Email: zhanghaiwen@amss.ac.cn

S07-2 流体力学方程的数学理论和数值方法

基于 IB/LS 方法的“左心室-血液”FSI 数值模拟

蔡力, 王永恒⁶⁹

Abstract: 浸入边界 (Immersed boundary, IB) 法是一种处理流固耦合问题的有效方法, 其思想就是将浸没在流体中的结构体视为一种特殊的流体, 通过在 Navier-Stokes 方程中加入力源项模拟结构体对流体的作用, 而流体对结构体的影响则通过速度来体现, 因而能够有效地处理含有复杂形状的结构体的流固耦合问题。水平集 (Level Set, LS) 方法在追踪运动界面方面具有显著优势, 对于满足 neo-Hookean 本构关系的结构体, 易于推导出相应的力源项。将浸没边界法与水平集方法结合, 得到 IB/LS 方法, 用于模拟心动周期内左心室-血液耦合系统的流体结构响应。

基于通量分裂思想的时空高精度紧致格式

陈艺冰⁷⁰

Abstract: 本文将基于通量分裂思想的时空高精度格式 HFVS[1] 进一步推广, 结合 HWENO 方法 [2], 获得一种求解双曲守恒律的时空高精度紧致格式。首先, 与传统 HWENO 格式相同, 引入关于守恒量空间导数的方程, 组成新的双曲型方程组; 其次, 利用单元守恒量及其导数, 采用 HWENO 重构技术, 获得每个单元中关于守恒量的高阶多项式及其各阶导数; 最后, 对新的双曲型方程组采用 HFVS 格式进行离散。与原 HFVS 采用了 WENO 重构技术来计算空间导数不同, 此时在 Lax-Wendroff 过程中所用到的空间导数是通过 HWENO 重构技术得到的, 因而格式变得紧致; 另一方面, 新的格式可以保证时空一致高精度, 避免了传统 HWENO 方法在时间上采用 Runge-Kutta 方法而遇到精度障碍的不足。本文最后给出多个典型数值算例, 数值结果证实了新的时空高精度紧致格式的良好效果。

浅水波方程的基于静水重构的间断 Galerkin 方法

李刚⁷¹

Abstract: 由于水体底部不平而带有几何源项的浅水波方程能够保持定常解。离散状态下, 能保持该定常解的数值方法被称为 well-balanced 方法, 该方法可以保持定常解至机器精度, 同时可以基于较粗网格来捕捉定常解的小扰动, 从而节约计算成本, 更加具有现实意义。这里, 针对浅水波方程, 我们基于静水重构思想以及分裂算法建立了 well-balanced 间断 Galerkin 方法。严格的数值分析以及广泛的数值试验均表明该方法保持 well-balanced 性质。此外, 数值结果表明该方法亦保持高阶精度与高分辨。

⁶⁹蔡力, 西北工业大学理学院应用数学系. Email: caili@nwpu.edu.cn

⁷⁰陈艺冰, 北京应用物理与计算数学研究所. Email: chen_yibing@iapcm.ac.cn

⁷¹李刚, 青岛大学数学与统计学院. Email: gangli1978@163.com

A free energy-based surface tension force model for simulation of multiphase flows by level-set method

袁海专⁷²

Abstract: A free energy-based surface tension force (FESF) model is presented for accurately resolving the surface tension force in numerical simulation of multiphase flows by the level set method. By using the analytical form of order parameter along the normal direction to the interface in the phase-field method and the free energy principle, FESF model offers an explicit and analytical formulation for the surface tension force. The only variable in this formulation is the normal distance to the interface, which can be substituted by the distance function solved by the level set method. On one hand, as compared to conventional continuum surface force (CSF) model in the level set method, FESF model introduces no regularized delta function, due to which it suffers less from numerical diffusions and performs better in mass conservation. On the other hand, as compared to the phase field surface tension force (PFSF) model, the evaluation of surface tension force in FESF model is based on an analytical approach rather than numerical approximations of spatial derivatives. Therefore, better numerical stability and higher accuracy can be expected. Various numerical examples are tested to validate the robustness of the proposed FESF model. It turns out that FESF model performs better than CSF model and PFSF model in terms of accuracy, stability, convergence speed and mass conservation. It is also shown in numerical tests that FESF model can effectively simulate problems with high density/viscosity ratio, high Reynolds number and severe topological interfacial changes.

Compact WENO Limiters for Discontinuous Galerkin Methods

钟杏慧⁷³

Abstract: Discontinuous Galerkin method is a class of finite element methods that has gained popularity in recent years due to its flexibility for arbitrarily unstructured meshes, with a compact stencil, and with the ability to easily accommodate arbitrary h-p adaptivity. However, some challenges still remain in specific application problems. In this talk, we design compact limiters using weighted essentially non-oscillatory (WENO) methodology for DG methods solving conservation laws, with the goal of obtaining a robust and high order limiting procedure to simultaneously achieve uniform high order accuracy and sharp, non-oscillatory shock transitions. The main advantage of compact limiters is their simplicity in implementation, especially on multi-dimensional unstructured meshes.

⁷²袁海专, 湘潭大学数学与计算科学学院. Email: yhz@xtu.edu.cn

⁷³钟杏慧, 浙江大学数学科学学院.

S08-2 无界域数学物理方程的数值方法及其应用

Robust integral formulations for electromagnetic scattering from three-dimensional cavities赖俊⁷⁴

Abstract: Scattering from large, open cavity structures is of importance in a variety of electromagnetic applications. We propose a new well-conditioned integral equation for scattering from general open cavities embedded in an infinite, perfectly conducting half-space. The integral representation permits the stable evaluation of both the electric and magnetic field, even in the low-frequency regime, using the continuity equation in a post-processing step. We establish existence and uniqueness results, and demonstrate the performance of the scheme in the cavity-of-revolution case. High-order accuracy is obtained using a Nyström discretization with generalized Gaussian quadratures.

A-stable time discretizations preserves maximal parabolic regularity李步扬⁷⁵

Abstract: It is shown that for a parabolic problem with maximal L^p -regularity (for $1 < p < \infty$), the time discretization by a linear multistep method or Runge-Kutta method has maximal L^p -regularity uniformly in the stepsize if the method is A-stable. In particular, the implicit Euler method, the Crank-Nicolson method, the second-order backward difference formula, and the Radau IIA and Gauss Runge-Kutta methods of all orders preserve maximal regularity. The $A(\alpha)$ -stable higher-order BDF methods have maximal L^p -regularity under an R -boundedness condition in a larger sector. These results are also extended to time-stepping methods for time-fractional evolution equations, including the L1 scheme, convolution quadratures generated by the A-stable BDFs, explicit Euler method, and the fractional version of the Crank-Nicolson method.

⁷⁴ 赖俊, 浙江大学数学科学学院. Email: laijun6@zju.edu.cn

⁷⁵ 李步扬, 香港理工大学数学系. Email: buyang.li@polyu.edu.hk

Asymptotic boundary conditions for periodic waveguides

陆雅言⁷⁶

Abstract: Currently there exist a variety techniques for simulating waves in unbound domains. The problem becomes more difficult when the physical domain extends to infinity periodically. In some cases, it is possible to write down an exact boundary condition at an artificial boundary (for truncating the unbounded domain) using proper nonlocal operators. These boundary conditions work extremely well for 2D problems, where the artificial boundary is one-dimensional. However, the boundary conditions involving nonlocal operators become too expensive for 3D problems. In the case of periodic waveguides, the number of propagating modes is usually finite. Therefore, away from local distortions, the wave field can be approximated by a sum of incoming and outgoing propagating modes. We have derived an asymptotic boundary condition based on this approximation. In this work, we analyze this boundary condition and consider its practical implementations. This is a joint work with HU, Zhen of Hohai University.

无界区域非线性 Dirac 孤波的计算及稳定性分析

邵嗣烘⁷⁷

Abstract: 非线性 Dirac 方程是量子物理中重要的方程之一，其孤波解的稳定性也一直是人们研究的热点。通过结合算子分裂方法和 Hermite 谱方法，我们给出了无界区域上非线性 Dirac 方程的数值模拟方法，并基于此方法讨论了非线性 Dirac 孤波解的稳定性。数值结果揭示了该稳定性与非线性指数及频率之间呈单调关系。最后通过引入解的稳定性系数，从理论上给出了部分佐证。

⁷⁶陆雅言, 香港城市大学数学系. Email: mayylu@cityu.edu.hk

⁷⁷邵嗣烘, 北京大学数学科学学院. Email: sihong@math.pku.edu.cn

S11-2 最优化专题

Nonnegative Tensor Factorizations Using an Alternating Direction Method蔡邢菊⁷⁸

Abstract: The nonnegative tensor (matrix) factorization finds more and more applications in various disciplines including machine learning, data mining, and blind source separation, etc. In computation, the optimization problem involved is solved by alternating minimizing one factor while the others are fixed. To solve the subproblem efficiently, we first exploit a variable regularization term which makes the subproblem far from ill-condition. Second, an augment Lagrangian alternating direction method is employed to solve this convex and well-conditioned regularized subproblem, and two accelerating skills are also implemented. Some preliminary numerical experiments are performed to show the improvements of the new method.

A descent cautious BFGS method for computing US-eigenvalues of symmetric complex tensors白敏茹⁷⁹

Abstract: US-eigenvalues of symmetric complex tensors and U-eigenvalues for non-symmetric complex tensors are very important because of their background of quantum entanglement. They are closely related to the best complex rank-one approximations to higher-order tensors. The problem of finding US-eigenpairs can be regarded as an unconstraint nonlinear optimization problem with complex variables, their complex conjugate variables and real variables. Optimization methods of this kind of problem often need a first- or second-order derivative of the objective function. However, such methods cannot be applied to real valued functions of complex variables because they are not necessarily analytic in their argument. In this paper, we first prove that the number of US-eigenvalues of a symmetric complex tensor is finite. Then, we study how to find US-eigenvalues of a symmetric complex tensor. We establish the first order complex Taylor series and Wirtinger calculus of complex gradient of real-valued functions with complex variables, their complex conjugate variables and real variables. Based on this theory, we propose a norm descent cautious BFGS method for computing US-eigenpairs of a symmetric complex tensor. The global and superlinear convergence of the proposed method are established. As an application, we give a method to compute U-eigenpairs for a non-symmetric complex tensor by finding the US-eigenpairs of its symmetric embedding. The numerical examples are presented to support the theoretical findings.

⁷⁸ 蔡邢菊, 南京师范大学. Email: caixingju@njnu.edu.cn⁷⁹ 白敏茹, 湖南师范大学. Email: minru-bai@163.com

张量最佳秩一逼近的神经网络算法

魏益民⁸⁰

Abstract: This talk presents the neural dynamic network to compute a best rank-one approximation of a real-valued tensor. We implement the neural network model by the ordinary differential equation (ODE), which is a class of continuous-time recurrent neural network. Several properties of solutions for the neural network are established. We prove that the local asymptotic stability of solutions for ODE by establishing an appropriate Lyapunov function under mild conditions. Furthermore, we also consider how to use the proposed neural networks for solving the tensor eigenvalue problem including the tensor H-eigenvalue problem, the tensor Z-eigenvalue problem, and the generalized eigenvalue problem with symmetric-definite tensor pairs. Finally, we generalize the proposed neural networks to the computation of the restricted singular values and the associated restricted singular vectors of real-valued tensors. We illustrate and validate theoretical results via numerical simulations.

S13-2 生命科学中的计算数学

Phase field modeling of Cell Polarity and Cell Delamination

张磊⁸¹

Abstract: Control of cellular behaviors plays a critical role in pattern formation, growth regulation and regeneration. Numerous developmental processes have been extensively studied from a mechanistic perspective, but only recently have serious efforts been directed toward systems biology approach. In this talk, I will present two biological systems to study pattern formation by using phase field model. First, we present a mathematical model that incorporates the interplays between Rac, filamentous actin (F-actin), and membrane tension for the formation of cell polarity. Second, I present a phase field approach to study the neuroblast delamination in *Drosophila*. Dynamics of cell ingression and role of actin-myosin network in apical constriction reveal that the myosin signaling drives neuroblast delamination in such rare event. The joint work with Feng Liu (PKU), Yan Yan (HKUST).

⁸⁰ 魏益民, 复旦大学. Email: ymwei@fudan.edu.cn

⁸¹ 张磊, 北京大学.

Inferring biological networks with strong associations by information theoretic approaches

李铁军⁸²

Abstract: Partial correlation (PC) or conditional mutual information (CMI) is widely used in detecting direct dependencies between the observed variables in a network by eliminating indirect correlations/associations, but it fails whenever there are some strong correlations in the network, due to the inherent underestimation problem of PC/CMI. We theoretically develop a multiscale association analysis to overcome this difficulty. Specifically, we first show why conditional mutual information (CMI)/partial correlation (PC) suffers from an underestimation problem for biological networks with strong correlations. Then, we propose a new measure, partial association (PA), based on the multiscale conditional mutual information (MCMI), to solve this problem. We show that linear PA and nonlinear PA can quantify the direct associations in biological networks in an accurate manner from both theoretical and computational aspects. Both simulated models and real datasets demonstrate that PA is superior to PC and CMI in terms of efficiency and effectiveness. We will also mention some new ideas still in progressing.

A probability polling state of neuronal systems underlying maximum entropy coding principle

周栋焯⁸³

Abstract: The maximum entropy principle is widely used in diverse fields. We address the issue of why the second order maximum entropy model, by using only firing rates and second order correlations of neurons as constraints, can well capture the observed distribution of neuronal firing patterns in many neuronal networks, thus, conferring its great advantage in that the degree of complexity in the analysis of neuronal activity data reduces drastically from $O(n^2)$ to $O(n)$, where n is the number of neurons under consideration. We first derive an expression for the effective interactions of the n -th order maximum entropy model using all orders of correlations of neurons as constraints and show that there exists a recursive relation among the effective interactions in the model. Then, via a perturbative analysis, we explore a possible dynamical state in which this recursive relation gives rise to the strengths of higher order interactions always smaller than the lower orders. Both numerical simulations and experimental data demonstrate the existence of such dynamical state in neuronal network dynamics. Finally, we invoke this hierarchy of effective interactions to provide a possible mechanism underlying the success of the second order maximum entropy model.

⁸² 李铁军, 北京大学.

⁸³ 周栋焯, 上海交通大学.

T01-2 微分方程数值计算及应用

The equilibrium melting path of the hexagonal ice.Han Wang⁸⁴

Abstract: Water is one of the most common materials on earth, but the understanding of the microscopic mechanism of the ice melting is still lacking. The ice melting is a typical rare event: the time spend by the system in the ice state is orders of magnitude longer than the transition time to the liquid state, which leads to a substantial difficulty for the microscopic simulation techniques like the molecular dynamics simulation. In this talk, the computation of the equilibrium melting path is made possible by coupling the string method with the molecular dynamics. We investigate the microscopic mechanism of the formation of the liquid nucleus in the bulk hexagonal ice, and disclose a different scenario from the classical nucleation theory at the early stage of the melting. The new techniques that accelerate the molecular dynamics simulation are also introduced in this talk.

Glassy dynamics, spinodal fluctuations, and the kinetic limit of nucleation in suspensions of colloidal hard rods倪冉⁸⁵

Abstract: Using simulations we identify three dynamic regimes in supersaturated isotropic fluid states of short hard rods: (i) for moderate supersaturations, we observe nucleation of multi-layered crystalline clusters; (ii) at higher supersaturation, we find nucleation of small crystallites which arrange into long-lived locally favored structures that get kinetically arrested; and (iii) at even higher supersaturation, the dynamic arrest is due to the conventional cage-trapping glass transition. For longer rods we find that the formation of the (stable) smectic phase out of a supersaturated isotropic state is strongly suppressed by an isotropic-nematic spinodal instability that causes huge spinodal-like orientation fluctuations with nematic clusters diverging in size. Our results show that glassy dynamics and spinodal instabilities set kinetic limits to nucleation in highly supersaturated hard-rod fluids.

⁸⁴ 王涵, 北京应用物理与计算数学研究所. Email: wang_han@iapcm.ac.cn

⁸⁵ 倪冉, Nanyang Technological University. Email: r.ni@ntu.edu.sg

应用 Born 自能修正的 Poisson-Nernst-Planck 模型研究 Kcsa 钾离子通道的选择性

刘雪娇⁸⁶

Abstract: 对于带相同电荷量的钠钾离子, 钾离子通道对尺寸大的钾离子表现出很强的通过性, 反而拒绝尺寸更小的钠离子通过。用于描述电扩散过程的传统 Poisson-Nernst-Planck (PNP) 理论不能对上述问题给出解释。主要原因在于, 传统的 PNP 模型把离子当做连续的点电荷分布, 而不考虑离子的尺寸信息, 从而不能区分出带相同电荷量的钠钾离子。为了研究尺寸选择性现象及其机制, 我们发展了一个考虑离子水化能的修正 PNP 模型 (BPNP), 并对 Kcsa 钾离子通道进行有限元模拟。基于三维自适应有限元并行开发平台 PHG 来求解 BPNP 方程, 数值计算结果表明, 新的 BPNP 模型可以从 Kcsa 通道内的浓度和电流两方面区分出钠钾离子, 表现出很强的钾离子选择性。

⁸⁶刘雪娇, 中国科学院数学与系统科学研究院. Email: liuxuejiao@lsec.cc.ac.cn

T03-2 优化、控制及反问题

Optimized Schwarz methods for the optimal control of systems governed by elliptic partial differential equationsYingxiang Xu, Xin Chen⁸⁷

Abstract: In the literature [A domain decomposition method with coupled transmission conditions for the optimal control of systems governed by elliptic partial differential equations, SIAM J. Numer. Anal., 33(6) 1996: 2401-2416], Benamou proved the convergence of a nonoverlapping Schwarz domain decomposition (DD) method with various Robin type transmission conditions. However, to achieve the possibly best performance of the DD method, the free parameters involved in these transmission conditions should be further optimized, which is the central idea of the well known Optimized Schwarz Methods (OSMs) that have been shown their efficiency in many applications. In this talk, we analyze in detail the OSMs for the optimal control of systems governed by elliptic partial differential equations without constraint. We drive first the transparent boundary conditions on the interface, which highlights us in the design of various local transmission conditions, including those mentioned by Benamou, the variants of the second order and the two-sided types applied in OSMs for second order elliptic PDEs. We then through optimizing the corresponding convergence factors to determine the asymptotically best transmission parameters for each kind of transmission conditions and derive the corresponding asymptotic convergence rate estimates. We find that the weight parameter enters both the predicted transmission parameters and the asymptotic convergence rate estimates. We find as well that the weight parameter plays an important role on the performance of the OSMs: the smaller the weight parameter is, the faster the OSMs converge. While when the weight parameter goes to infinity, we arrive at the results for solving a biharmonic problem using mixed form. We use numerical experiments to validate the theoretical findings.

The Eigenvalue Optimization Problem in Quantum Dots郭双冰, 李订芳, 张志跃, 吕锡亮⁸⁸

Abstract: In this paper, we study the optimization algorithm for the first eigenvalue of schrodinger operator under volume constraints. We show that the solution to the optimization problem is a fixed point of the systems. The error of the Finite element discretization is established. We also provide that the error estimate for the numerical solution. A monotonic decreasing algorithm is presented to solve the eigenvalue optimization problem. Numerical simulations demonstrate the efficiency of the method.

⁸⁷ 徐英祥, 东北师范大学数学与统计学院. Email: yxxu@nenu.edu.cn⁸⁸ 郭双冰, 河南科技学院. Email: iceflyingsouth@163.com

An efficient error estimation for model order reduction of parametrized evolution equations

张永金⁸⁹

Abstract: In this talk we present an a posteriori output error bound for model order reduction of parametrized evolution equations. With the help of the dual system and a simple representation of the relationship between the field variable error and the residual of the primal system, a sharp output error bound is derived. Such an error bound successfully avoids the accumulation of the residual over time, which is a common drawback in the existing error estimations for time-stepping schemes. An estimation needs to be performed for practical computation of the error bound, and as a result, the output error bound reduces to an output error estimation. The proposed error estimation is applied to several kinds of problems and the numerical experiments demonstrate the performance and efficiency of the proposed error estimation.

T05-1 谱方法、数值逼近与计算几何

A robust algorithm for the inversion of Laplace transform using Puiseux expansion

Wang Tongke, Gu Yuesheng, Zhang Zhiyue⁹⁰

Abstract: This paper is devoted to designing a practical algorithm to invert the Laplace transform by assuming that the transform possesses the Puiseux expansion at infinity. First, the general asymptotic expansion of the inverse function at zero is derived, which can be used to approximate the inverse function when the variable is small. Second, an inversion algorithm is formulated by splitting the Bromwich integral into two parts. One is the main weakly oscillatory part, which is evaluated by a composite Gauss-Legendre rule and its Kronrod extension, and the other is the remaining strongly oscillatory part, which is integrated analytically using the Puiseux expansion of the transform at infinity. The algorithm is accurate and robust, and can be implemented automatically. Finally, some typical Laplace transforms are performed to show that the algorithm can be used to invert a wide range of Laplace transforms automatically with high accuracy and the output error estimator matches well with the true error.

⁸⁹张永金, 河南理工大学. Email: zhyj@hpu.edu.cn

⁹⁰王同科, 天津师范大学数学科学学院. Email: wangtke@sina.com

Fast convergence of generalized DeTemple sequences and the relation to the Zeta function

吴善和⁹¹

Abstract: In this work, we introduce new sequences which generalize the celebrated De-Temple sequence, having enhanced speed of convergence. We also obtain a new representation for Euler's constant in terms of the Riemann zeta function evaluated at positive odd integers. Our results extend and improve some earlier results in this direction.

一类二维 Cauchy 主值积分的近似计算

李金⁹²

Abstract: 对某一类二维 Cauchy 主值积分, 基于分片常数插值近似计算, 得到相应的超收敛现象。证明了超收敛阶, 数值算例验证了理论分析的有效性。

A Further Analysis of Backward Error in Polynomial Deflation

Min Wang⁹³

Abstract: When polynomial roots vary widely in order of magnitude, severe inaccuracy problem may occur due to deflation scheme. Peters and Wilkinson have proposed deflation schemes to prevent backward stability of later approximation from being worse compared to the one of deflated approximate root. In this presentation, I will show that this root structure can be utilized to help improve the backward stability of later approximate roots, when using deflation schemes.

⁹¹ 吴善和, 龙岩学院. Email: shanhely@126.com

⁹² 李金, 山东建筑大学. Email: lijin@lsec.cc.ac.cn

⁹³ 王敏, 复旦大学. Email: 15210180016@fudan.edu.cn

Fractional Hermite Interpolation Formulas for Non-smooth Functions

Jiayin Zhai (翟佳音), Zhiyue Zhang (张志跃)⁹⁴

Abstract: The interpolation of a function is the basic of the numerical computation. However, the highly approximation to non-smooth functions is a huge challenge in Science and Engineering. we devote to constructing the fractional Hermite interpolation formulas, which are based on local fractional Taylor expansions, for non-smooth functions. Firstly, the unique existence of the Hermite interpolation formulas is proved, and the corresponding explicit expressions and error remainders are derived. In addition, the convergent order of the piecewise hybrid interpolation, a combination of fractional-order Hermite interpolation and integer-order Hermite interpolation, is discussed. Finally, the typical numerical examples under different interpolation conditions are presented to show the high accuracy of the fractional Hermite interpolation method and verify the theoretical analysis.

T06-2 有限元和边界元方法

Multi-step inertial Krasnoselskii-Mann algorithm for nonexpansive mappings

董巧丽⁹⁵

Abstract: In this paper, I first introduce a multi-step inertial Krasnosel'skii-Mann algorithm for nonexpansive mappings, for which we present an exhaustive convergence analysis by using the bounded perturbation resilience. The obtained results can be applied to construct various multi-step inertial monotone operator splitting methods, including the multi-step inertial forward-backward splitting (MiFBS), the multi-step inertial gradient-projection method (MiGPM), the multi-step inertial Douglas-Rachford splitting (MiDRS), and the multi-step inertial primal-dual splitting method (MiPDS). We present the convergence conditions for the MiFBS, which are different with the existing results. The convergence properties of the MiDRS and MiPDS are first investigated.

⁹⁴ 翟佳音, 南京师范大学. Email: jiayinzhai@sina.com

⁹⁵ 董巧丽, 中国民航大学. Email: dongql@lsec.cc.ac.cn

Arbitrary Lagrangian-Eulerian discontinuous Galerkin method for conservation laws

夏银华⁹⁶

Abstract: In this talk, we present and analyze an arbitrary Lagrangian-Eulerian discontinuous Galerkin (ALE-DG) method with a time-dependent approximation space for conservation laws, which satisfies the geometric conservation law. For the semi-discrete ALE-DG method, when applied to nonlinear scalar conservation laws, a cell entropy inequality, L^2 stability and error estimates are proven. More precisely, we prove the sub-optimal $(k + \frac{1}{2})$ convergence for monotone fluxes, and optimal $(k + 1)$ convergence for an upwind flux, when a piecewise P^k polynomial approximation space is used. For the fully-discrete ALE-DG method, the geometric conservation law and the local maximum principle are proven. We also state conditions for slope limiters, which ensure total variation stability of the method.

一种求解三维 Neumann 边界条件线弹性问题线性二次有限元方程的并行高效预条件子

冯春生, 舒适⁹⁷

Abstract: 针对一种满足适定性条件的纯 Neumann 边界的三维线弹性问题的二次有限元离散代数系统, 研究其并行快速求解算法及解法器。首先, 讨论了二次有限元离散化代数系统的适定性, 数值实验表明二次有限元误差函数在 L^2 和 H^1 范数下均具有饱和误差阶。接着, 针对二次有限元代数系统给出了两类求解算法, 其中重点研究了两种基于 AMG 法和高斯赛德尔迭代法 (GS) 的组合型预条件子, 并研制了相应的预条件 GMRES(k) 解法器 (BAG-GMRES(k) 和 BvAG-GMRES(k))。数值实验验证了基于 AMG 的组合型预条件 GMRES(k) 法的迭代次数和求解时间均优于常用求解方法 ILU(0)-GMRES(k)。最后, 在上述串行预条件子算法解法器的基础上, 设计了相应的具有极小化数据通信的并行 AMG 法和 GS 的组合型预条件算法, 数值试验验证了该算法具有良好的扩展性。

⁹⁶夏银华, 中国科学技术大学. Email: yhxia@ustc.edu.cn

⁹⁷冯春生, 湘潭大学. Email: spring@xtu.edu.cn

SDFEMs on Triangular Meshes for Convection-dominated Problems

张进⁹⁸

Abstract: In this talk, we will present some recent developments in streamline diffusion finite element methods (SDFEMs) on triangular meshes for convection-dominated problems. A series of integral inequalities on triangular meshes are derived, which are essential for estimates of diffusion and convection terms. Based on these inequalities, we analyze the superconvergence behavior of SDFEMs, which reveals the differences between linear SDFEMs and bilinear ones. With the help of weighted estimates, these superconvergence results yield optimal order L^2 errors. In the meantime, the above results provide a clue for choices of linear and bilinear elements in exponential layers and characteristic layers.

Virtual Element Method for Linear Elasticity Problem in Mixed Weakly Symmetric Formulation

张百驹, 冯民富⁹⁹

Abstract: We propose and analyze a virtual element method for linear elasticity problem in mixed weakly symmetric formulation, that is to say, stresses are not required to be symmetric, but only to satisfy a weaker condition based on Lagrange multipliers. The proposed method is well-posed, and the error bounds are shown to be uniform with the incompressibility parameter λ . Numerical tests confirm the convergence rate that is expected from the theory.

⁹⁸张进, 山东师范大学. Email: jinzhangalex@sdu.edu.cn

⁹⁹张百驹, 四川大学数学学院. Email: 164170437@qq.com

T09-2 分数阶方程

A Fractional Order Collocation Method for Second Kind Volterra Integral Equations with Weakly Singular KernelsHaotao Cai and Yanping Chen¹⁰⁰

Abstract: In this paper, we develop a fractional order spectral collocation method for solving second kind Volterra integral equations with weakly singular kernels. It is well known that the original solution of second kind Volterra integral equations with weakly singular kernels usually can be split into two parts, the first is the singular part and the second is the smooth part with the assumption that the integer m being its smooth order. On the basis of this characteristic of the solution, we first choose the fractional order Lagrange interpolation function of Chebyshev type as the basis of the approximate space in the collocation method, and then construct a simple quadrature rule to obtain a fully discrete linear system. Consequently, with the help of the Lagrange interpolation approximate theory we establish that the fully discrete approximate equation has a unique solution for sufficiently large n , where $n + 1$ denotes the dimension of the approximate space. Moreover, we prove that the approximate solution arrives at an optimal convergence order $\mathcal{O}(n^{-m} \log n)$ in the infinite norm and $\mathcal{O}(n^{-m})$ in the weighted square norm. In addition, we prove that for sufficiently large n , the infinite condition number of the coefficient matrix corresponding to the linear system is $\mathcal{O}(\log^2 n)$ and its spectral condition number is $\mathcal{O}(1)$. Numerical examples are presented to demonstrate the effectiveness of the proposed method.

¹⁰⁰ 蔡好涛, 山东财经大学. Email: caihaotao@126.com

Fast evaluation and high accuracy finite element approximation for the time fractional subdiffusion equation

任金城, 毛士鹏, 张继伟¹⁰¹

Abstract: In this talk, an efficient algorithm for the evaluation of the Caputo fractional derivative and the superconvergence property of fully discrete finite element approximation for the time fractional subdiffusion equation are considered. First, the space semidiscrete finite element approximation scheme for the constant coefficient problem is derived and supercloseness result is proved. The time discretization is based on the L_1 -type formula, whereas the space discretization is done using finite element method, the fully discrete scheme is developed. Under some regularity assumptions, the superconvergence estimate is proposed and analyzed. Then extension to the case of variable coefficients is also discussed. To reduce the computational cost, the fast evaluation scheme of the Caputo fractional derivative to solve the fractional diffusion equations is designed. Finally, numerical experiments are presented to support the theoretical results.

Orthogonal spline collocation method for fourth-order fractional evolution equation

杨雪花¹⁰²

Abstract: The L_1 orthogonal spline collocation (L1-OSC) method is presented for fourth-order fractional evolution equation, which arises in a number of applications, most notably the viscoelastic materials, e.g., flow in heterogeneous media. The stability of the L1-OSC method is proved. We also exhibit the priori error estimates in the L_2 , L^∞ , and H^1 -norms. Besides, we provide some numerical experiments to demonstrate the results of theoretical analysis and show the accuracy and effectiveness of the L1-OSC method.

¹⁰¹ 任金城, 河南财经政法大学. Email: renjincheng2001@126.com

¹⁰² 杨雪花, 北京计算物理与应用数学研究所. Email: hunanshidayang@163.com

The extrapolated Crank-Nicolson OSC method for a nonlinear fractional Cable equation with nonlinear variable coefficient

张海湘¹⁰³

Abstract: 1) We construct ENC OSC methods for the numerical solution nonlinear fractional Cable equation with nonlinear variable coefficient in two space variables. (2) Based on the idea of weighted and shifted Grunwald difference operator, we establish ENC OSC schemes with temporal accuracy order equal to two. (3) We prove proposed ENC OSC methods are second order accurate in time and of optimal order in certain $H_j(j = 0, 1)$ norms in space. Moreover, because the nonlinear fractional Cable equation involve multi-term fractional order operators and nonlinear variable coefficient, its stability and convergence analysis become more perplexing to handle. We introduce some new techniques to derive the convergence analysis. In particular, we present a new scheme for the selection of u_h^1 so that we can get the desired second order global error estimate in time,.

Optimal error analysis of a direct discontinuous Galerkin method for time-fractional reaction-diffusion equation

Chaobao Huang, Martin Stynes¹⁰⁴

Abstract: In this work, a fully discrete DDG method for the time-fractional reaction-diffusion equation with Dirichlet boundary condition is proposed. The proposed method is based on the finite difference scheme in temporal and DDG method in spatial. The L_2 norm stability result is given for the proposed method. By constructing a new projection P to handle the Dirichlet boundary condition, the L_2 norm convergence result is derived. Finally, numerical examples are present to demonstrate the theoretical convergence results.

Regularity and spectral methods for two-sided fractional differential equations with a low order

郝朝鹏¹⁰⁵

Abstract: We study regularity and numerical methods for two-sided fractional diffusion equations with a lower-order term. We show that the regularity of the solution in weighted Sobolev spaces can be greatly improved compared to that in standard Sobolev spaces. With this regularity, we improve higher-order convergence of a spectral Galerkin method. We propose a spectral Petrov-Galerkin method and provide an optimal error estimate for the Petrov-Galerkin method. Numerical results are presented to verify our theoretical convergence orders.

¹⁰³ 张海湘, 湖南工业大学. Email: hassenzhang@163.com

¹⁰⁴ 黄朝宝, 北京计算科学研究中心. Email: huangcb@csrc.ac.cn

¹⁰⁵ 郝朝鹏, 东南大学数学学院. Email: haochpeng@126.com

分会场报告 3

S01-1 PDE 并行、快速算法研究进展

非结构网格粒子输运问题的并行计算

刘杰¹⁰⁶

Abstract: 粒子输运理论是研究微观粒子(中子、光子、电子)在介质中迁移统计规律的数学理论,广泛应用于模拟核临界态、核反应堆、放射性治疗等领域的物理现象。本报告介绍我们在非结构网格粒子输运问题的并行计算方面的研究成果和进展。设计了基于网格划分的非结构网格粒子输运 Sn 并行算法框架,实现了多个角方向和多个能群的同时计算,可以根据计算机系统系统的通信性能动态地调整通信的粒度。综合考虑了所有方向和所有网格点的数据依赖关系,设计了一种优先级排序计算方法,优先计算需要数据发送和非接收数据的计算任务,达到计算与通信重叠的目的。在能群和角方向上设计了 OpenMP 共享并行计算方法,实现了非结构粒子输运问题的 MPI+OpenMP 混合并行计算,在银河高性能计算机系统上进行了性能优化和测试。

计算电磁学中矩量法的复数稠密矩阵方程问题研究

张玉¹⁰⁷

Abstract: 矩量法是经典的电磁场数值分析方法之一,具有较高的理论精度。矩量法的核心技术问题是如何构建矩阵方程、如何求解大型复数稠密矩阵方程。围绕这些问题,本报告介绍基于神威蓝光、天河二号等超级计算机的大规模并行矩量法的矩阵填充技术以及复数稠密矩阵的 LU 分解并行策略,并给出矩量法在机载雷达布局、目标隐身特性、导弹瞄准线等系统级精确电磁仿真难题中的应用。

¹⁰⁶刘杰,国防科学技术大学. Email: liujie@nudt.edu.cn

¹⁰⁷张玉,西安电子科技大学. Email: yuzhang@mail.xidian.edu.cn

面向复杂应用数值模拟的自适应预条件策略

徐小文¹⁰⁸

Abstract: 对于复杂应用的大规模数值模拟, 现有预条件算法的效率受到应用特征与机器体系结构特征带来的双重挑战。一方面, 多物理耦合、多介质、多尺度、强非线性等复杂应用特征越来越显著, 影响算法的收敛速度, 另一方面, 计算机体系结构越来越复杂, 多级嵌套海量并行与异构协同的发展趋势日益明显, 影响其并行可扩展性。一个好的预条件策略需要同时兼顾收敛性与并行性, 综合考虑计算与通信的权衡。在实际复杂应用的长时间积分模拟中, 单个算法或算法的某组特定参数很难保证对所有系统都达到最优或有效求解。本报告尝试提出一种自适应预条件策略, 该策略针对时间积分过程方程组序列中矩阵性质的相似性与差异, 基于预条件算法的计算与通信比分析, 结合残差的后验评估, 可以在数值模拟过程自适应地选择和切换预条件算法的组件和参数, 以期望达到良好的整体求解效率。报告将以多重网格算法为例, 通过设计自适应光滑与粗化策略, 表明该思路的可行性, 并给出在实际数值模拟大规模计算中的应用实例。

具有多重小周期构造的复合材料结构热传导问题的高阶三尺度方法

杨自豪¹⁰⁹

Abstract: 非均质材料具有嵌套式多尺度的内在特征, 材料特性与响应体现在从微观到细观直至宏观的不同尺度范围中, 研究非均质材料的多尺度耦合方法为材料与结构的一体化设计提供理论依据。本文针对具有双重小周期构造的复合材料热传导问题, 给出了一种微-细-宏观一体化分析的高阶三尺度计算方法, 并针对典型问题进行了数值模拟。构造了微观单胞函数、细观单胞函数以及交叉项单胞函数族, 建立了等效材料参数的升尺度计算模型, 最终构造了温度场以及热流密度场的高阶三尺度渐进展开式, 并给出了多尺度有限元算法。数值结果表明, 使用高阶三尺度方法预测具有多重小周期构造的复合材料热传导性能是有效的。

热传导方程的并行有限体积格式

盛志强¹¹⁰

Abstract: 我们针对任意多边形网格上的热传导方程, 设计了具有保正性的并行有限体积格式。首先给出内边界上的预估值, 然后在子区域上分别采用隐式保正有限体积格式计算子区域内部的值, 最后采用隐式保正有限体积格式校正内边界上的值。我们的算法只需要局部通讯, 算法的可扩展性非常好。数值实验显示, 该并行格式在精度、稳定性和并行效率等方面都取得了令人满意的结果。

¹⁰⁸ 徐小文, 北京应用物理与计算数学研究所. Email: xwxu@iapcm.ac.cn

¹⁰⁹ 杨自豪, 西北工业大学. Email: yangzihao@nwpu.edu.cn

¹¹⁰ 盛志强, 北京应用物理与计算数学研究所. Email: sheng_zhiqiang@iapcm.ac.cn

S03-1 界面问题的建模与计算

Invariant Energy Quadratization Approach for Incompressible Smectic-A Liquid Crystal Flow张辉¹¹¹

Abstract: In this talk, we construct the first-order decoupled and the second-order coupled temporal accurate energy stable schemes to solve the smectic-A liquid crystals model in the incompressible fluid. This model involves the incompressible Navier-Stokes equation and a fourth order phase-field equation for the order parameter of smectic-A liquid crystals. The projection method is adopted to decouple the pressure and the velocity in the Navier-Stokes equation. Moreover, the invariant energy quadratization method is used to linear the nonlinear functionals, meanwhile preserving the energy stability. Then we present the fully discrete energy stable schemes by using finite differences in time and C^0 -finite elements in space where the fourth order equation shall be transformed into two second order equations. At last we calculate several numerical tests to illustrate the temporal accuracy of the proposed schemes and verify that our schemes are unconditionally energy stable. Moreover, we simulate the process of undulation in the smectic-A liquid crystals under the effect of the shear flows and the magnetic field, which is consistent with other works.

¹¹¹张辉, 北京师范大学.

High order energy stable and efficient local discontinuous Galerkin methods for the phase field models

徐岩¹¹²

Abstract: The goal of this talk is to propose energy stable fully discrete local discontinuous Galerkin (LDG) finite element methods for the phase field models. Based on the method of lines, we first construct an LDG method and prove the semi-discrete energy stability. Then, we develop a first order and a second order semi-implicit convex splitting schemes based on a convex splitting principle of the discrete Cahn-Hilliard energy, and prove the corresponding unconditional energy stabilities. In addition, a semi-implicit spectral deferred correction (SDC) method combining the first order convex splitting scheme is employed to improve the temporal accuracy. The SDC method is high order accurate and stable numerically with the time step proportional to the spatial mesh size. The resulting algebraic equations at the implicit level are nonlinear. Due to the local properties of the LDG methods, the resulting implicit scheme is easy to implement and can be solved in an explicit way when it is coupled with iterative methods. An efficient nonlinear multigrid method are used to solve the equations. Numerical experiments of the accuracy and long time simulations are presented to illustrate the high order accuracy in both time and space, the capability and efficiency of the proposed methods.

Efficient and accurate Fourier approximations of nonlocal phase-field equations

杨将¹¹³

Abstract: This work is concerned with the spectral methods for the numerical approximation of integral differential equation models associated with some linear nonlocal diffusion operators with periodic boundary conditions. For radially symmetric kernels, the nonlocal operators under consideration are diagonalizable in Fourier space. A challenge is the accurate and fast evaluation of the Fourier symbols which consist of possibly singular and highly oscillatory integrals. For a large class of fractional power-like kernels, we propose a new approach to reformulate the Fourier symbols as coefficients of a series expansion which correspond to solutions of some simple ODE models. We then propose a hybrid algorithm to provide fast evaluation of Fourier symbols in both one and higher dimensional spaces. As applications, we combine this hybrid spectral discretization in the spatial variables and fourth-order exponential time differencing Runge–Kutta for temporal discretization to approximate some nonlocal gradient flows including nonlocal Allen–Cahn equation, nonlocal Cahn–Hilliard equation, and nonlocal phase-field crystal models. Numerical results show the accuracy and effectiveness of this fully discrete schemes and illustrate some interesting phenomena associated with the nonlocal models.

¹¹² 徐岩, 中国科学技术大学. Email: yxu@ustc.edu.cn

¹¹³ 杨将, 美国哥伦比亚大学. Email: jyanghku@gmail.com

三维理想 MHD 方程的严格 divergence-free 非结构网格 DG 方法

郑伟英¹¹⁴

Abstract: 三维理想磁流体力学 (MHD) 方程组在空间等离子体和磁约束聚变等离子体中有广泛应用, 舒其望教授、邱建贤教授以及国内外学者在间断 Galerkin (DG) 方法的研究方面已经有了很多重要工作。磁场严格满足 divergence-free 条件的数值方法在磁流体的长时间模拟中对保持磁场结构非常重要, 近年来受到越来越多的关注, 李凤艳教授、徐立伟教授等人基于结构网格构造了严格 divergence-free 的 Central DG 方法。三维四面体网格上的 DG 方法在处理复杂几何结构时具有显著优势, 但由于其计算程序研制非常困难, 相关研究工作非常少。另外, 由于构造四面体网格的对偶网格极其困难, 使得 Central DG 方法很难推广到三维非结构网格上, 目前尚未见到三维 MHD 方程的非结构网格严格 divergence-free DG 方法。本工作基于三维四面体网格和分片线性多项式逼近, 提出了一种 MHD 方程组的严格 divergence-free DG 方法, 且具有 2 阶精度。我们将用多个算例显示方法的优点以及大规模并行计算的可扩展性。

Error estimates for a fully discretized scheme to a Cahn-Hilliard phase-field model for two-phase incompressible flows

蔡勇勇¹¹⁵

Abstract: We carry out in this paper a rigorous error analysis for a finite element discretization of the linear, weakly coupled energy stable scheme for a Cahn-Hilliard phase-field model of two-phase incompressible flows with matching density.

Recursive Integral Method For The Nonlinear Non-Selfadjoint Transmission Eigenvalue Problem

季霞¹¹⁶

Abstract: The transmission eigenvalue problem is an eigenvalue problem that arises in the scattering of time-harmonic waves by an inhomogeneous medium of compact support. Based on a fourth order formulation, the transmission eigenvalue problem is discretized by the Morley element. For the resulting quadratic eigenvalue problem, a recursive integral method is used to compute real and complex eigenvalues in prescribed regions in the complex plane. Numerical examples are presented to demonstrate the effectiveness of the proposed method.

¹¹⁴ 郑伟英, 中国科学院数学与系统科学研究院. Email: zwy@lsec.cc.ac.cn

¹¹⁵ 蔡勇勇, 北京计算科学研究中心. Email: yongyong.cai@csrc.ac.cn

¹¹⁶ 季霞, 中国科学院数学与系统科学研究院. Email: jixia@lsec.cc.ac.cn

S04-1 材料科学的可计算建模与计算方法**Density Functional Theory: Two Cases Study**陈景润¹¹⁷

Abstract: In the first part, we will discuss the convergence of the first linear-scaling method: Divide and Conquer method for Density Functional Theory (DFT) calculations, under gap conditions for both the global problem and local problems. We show by examples that both conditions are necessary. In the second part, we apply the many-body van der Waals (vdW) corrected DFT scheme to study a tip-substrate system at the nanoscale. In a loading-sliding process, the tip-substrate distance is found to be essential for nanofrictional behavior, through determining the competition between vdW contributions and electronic contributions. As the tip approaches the substrate, this competition results in a smooth transition of normal forces from attraction to repulsion, and the friction coefficient in turn undergoes a sign change from negativity to positivity with possible giant magnitudes and strong anisotropy.

An efficient algorithm for the Sternheimer equation in the GW approximation刘芳¹¹⁸

Abstract: In the Green's function formalism of a many-body perturbation theory, the excitation of the material is described in terms of quasi-particle energies (eigenvalues) of a single-particle Hamiltonian that contains a self energy term. We will talk about a computational issue in the GW approximation of the self-energy. The computation of dielectric matrix is important in the GW approximation. The standard method to compute dielectric matrix requires information of thousands of empty states which is very demanding. Hence an alternative method was proposed to overcome this problem by solving the so called Sternheimer equation. An efficient algorithm based on low rank approximation for solving the Sternheimer equation will be introduced.

¹¹⁷陈景润, 苏州大学.¹¹⁸刘芳, 中央财经大学. Email: fliu@lsec.cc.ac.cn

Extreme-Scale Phase Field Simulations of Coarsening Dynamics on the Sunway TaihuLight Supercomputer

张鉴¹¹⁹

Abstract: Many important properties of materials such as strength, ductility, hardness and conductivity are determined by the microstructures of the material. During the formation of these microstructures, grain coarsening plays an important role. The Cahn-Hilliard equation has been applied extensively to simulate the coarsening kinetics of a two-phase microstructure. It is well accepted that the limited capabilities in conducting large scale, long time simulations constitute bottlenecks in predicting microstructure evolution based on the phase field approach. We present here a scalable time integration algorithm with large stepsizes and its efficient implementation on the Sunway TaihuLight supercomputer. The highly nonlinear and severely stiff Cahn-Hilliard equations with degenerate mobility for microstructure evolution are solved at extreme scale, demonstrating that the latest advent of high performance computing platform and the new advances in algorithm design are now offering us the possibility to simulate the coarsening dynamics accurately at unprecedented spatial and time scales.

Deterministic Solvers for the Wigner Quantum Dynamics

邵嗣烘¹²⁰

Abstract: The Wigner function has provided an equivalent and convenient way to render quantum mechanics in phase space. A whole branch of experimental physics exists, known as quantum tomography, the purpose of which is reconstructing the Wigner function from measurements. Distinct from the Schrödinger equation, the most appealing feature of the Wigner equation, which governs the dynamics of the Wigner function, is that it shares many analogies to the classical mechanism and simply reduces to the classical counterpart when the reduced Planck constant vanishes. Despite the theoretical advantages, numerical resolutions for the Wigner equation is notoriously difficult and remains one of the most challenging problems in computational physics. The commonly used finite difference methods fail to capture the highly oscillatory structure accurately. We completed the design and implementation of a highly accurate numerical scheme for the Wigner quantum dynamics in 4D phase space. Our algorithm combines an efficient conservative semi-Lagrangian scheme in the temporal-spatial space with an accurate spectral element method in the momentum space. With it, the Wigner function for a one-dimensional Helium-like system was clearly shown for the first time.

¹¹⁹张鉴, 中国科学院计算机网络信息中心. Email: zhangjian@sccas.cn

¹²⁰邵嗣烘, 北京大学. Email: sihong@math.pku.edu.cn

Atomistic-to-continuum coupling method and its adaptivity

王皓¹²¹

Abstract: We give an introduction to atomistic-to-continuum coupling (a/c) method and its adaptivity. We give residual based error estimators for several different a/c methods and develop adaptive algorithms based on these estimators. The results are illustrated by numerical experiments and a brief outlook of this field is discussed.

On adaptive finite element simulations of high harmonic generation with time-dependent density functional theory

胡光辉¹²²

Abstract: High harmonic generation (HHG) plays an important role in the emerging attosec-ond physics, and has applications on developing novel techniques such as imaging of molecular orbitals. There are several challenges on numerical study of HHG. In this talk, HHG as well as theoretical and numerical challenges on its study will be introduced. Then a numerical framework of adaptive finite element solutions of Kohn-Sham and time-dependent Kohn-Sham equations for HHG simulations will be described in detail. Numerical results will show the effectiveness of the proposed method.

S05-1 Recent advances in nonstandard discretization methods in scientific and engineering computation

A nonconforming finite element method for an acoustic fluid-structure interaction problem

崔金涛¹²³

Abstract: In this talk we discuss a nonconforming finite element approximation of the vibration modes of an acoustic fluid-structure interaction. Displacement variables are used for both the fluid and the solid. The numerical scheme is based on the irrotational fluid displacement formulation; hence it is free of spurious eigenmodes. The method uses weakly continuous P1 vector fields for the fluid and classical piecewise linear elements for the solid; and it satisfies optimal order error estimates on properly graded meshes. The theoretical results are confirmed by numerical experiments.

¹²¹ 王皓, 四川大学. Email: wangh@scu.edu.cn

¹²² 胡光辉, 澳门大学. Email: garyhu@umac.mo

¹²³ 崔金涛, 香港理工大学. Email: jintao.cui@polyu.edu.hk

An optimal high-order locking-free finite element method for elastic vibration problems

黄建国¹²⁴

Abstract: In this talk, we are going to introduce a high-order locking-free finite element method for solving elastic vibration problems. In the time direction, the discretization is carried out using the continuous discontinuous Galerkin (CDG) method. The spatial discretization is based on nonconforming finite element methods satisfying some weak continuity. The theoretical analysis shows that the method can reach the optimal convergence order both in the time and the space directions, and the error estimates are independent of the Lamé coefficients.

Differential complex, Hemioltz decompositions and mixed methods

黄学海¹²⁵

Abstract: A framework to systematically construct differential complex and Helmholtz decompositions is developed. The Helmholtz decomposition is used to decouple the mixed formulation of high order elliptic equations into combination of Poisson-type and Stokes-type equations. By finding the underlying complex, this decomposition is applied in the discretization level to design fast solvers for solving the linear algebraic system. It can be also applied in the continuous level first and then discretize the decoupled formulation, which leads to a natural superconvergence between the Galerkin projection and the decoupled approximation. Examples include but not limit to: biharmonic equation, triharmonic equation, fourth order curl equation, HHJ mixed method for plate problem, and Reissner-Mindlin plate model etc. As a by-product, Helmholtz decompositions for many dual spaces are obtained.

A nonconforming finite element on polygonal meshes

汪艳秋¹²⁶

Abstract: A nonconforming lowest order Crouzeix-Raviart type finite element is constructed on polygonal meshes. Local construction in each polygon depends on whether the polygon has odd or even number of vertices. Because of this, the topological structure of connected regions consisting of polygons with even number of vertices plays an essential role in understanding the global finite element space. To analyze such topological structure, a new technique tool using the concept of cochain complex and cohomology is developed. Despite the seemingly complicated theoretical analysis, implementation of the element is straight-forward. The nonconforming finite element method has optimal a priori error estimates and supporting numerical results are presented.

¹²⁴ 黄建国, 上海交通大学. Email: jghuang@sjtu.edu.cn

¹²⁵ 黄学海, 温州大学. Email: xuehaihuang@gmail.com

¹²⁶ 汪艳秋, 南京师范大学. Email: yqwang@njnu.edu.cn

Efficient and accurate numerical solutions for the Helmholtz equation with high wave numbers

王坤¹²⁷

Abstract: In this talk, we introduce a kind of nonstandard discretization schemes based on rearranging the truncation error for solving the Helmholtz equation with high wave numbers. The most important result presented in this study is that the developed methods are pollution free in the cases considered, and their convergence orders are independent of the wave number k . The idea is also easily extended to other problems, such as the singular perturbation equations.

Convergence of adaptive mixed finite element methods for Hodge Laplacian equation: without harmonic forms

吴永科¹²⁸

Abstract: Finite element exterior calculus (FEEC) has been developed as a systematically framework for constructing and analyzing stable and accurate numerical method for partial differential equations by employing differential complexes. This paper is devoted to analyze the convergence of adaptive mixed finite element methods for Hodge Laplacian equations based on FEEC without considering harmonic forms. More precisely, a residual type *posteriori* error estimates is obtained by using the Hodge decomposition, the regular decomposition and bounded commuting quasi-interpolants. An additional marking strategy is added to ensure the quasi-orthogonality. Using this quasi-orthogonality, the uniform convergence of adaptive mixed finite element methods is obtained without assuming the initial mesh size is small enough. This is a joint work with Long Chen (UCI).

¹²⁷ 王坤, 重庆大学. Email: kunwang@cqu.edu.cn

¹²⁸ 吴永科, 电子科技大学. Email: wuyongke1982@sina.com

S09-1 Krylov 子空间算法及预处理技术

Preconditioned modified Hermitian and skew-Hermitian splitting iteration methods for the fractional nonlinear Schrödinger equations殷俊峰¹²⁹

Abstract: After discretized by an implicit conservative difference scheme, a complex linear equations with Toeplitz-like structure is obtained from the space fractional coupled nonlinear Schrödinger equations. A class of preconditioned modified Hermitian and skew-Hermitian splitting iteration method is proposed to solve the discretized linear system without complex arithmetic. Theoretical analyses show that the preconditioned modified Hermitian and skew-Hermitian splitting iteration methods are unconditionally convergent. From the view point of practical implementation, we give a special case of the preconditioned modified Hermitian and skew-Hermitian splitting iteration method and study in details the choices of the optimal parameters to minimized the upper bound of the spectral radius of iteration matrix. Numerical examples are given to further confirm the efficiency of our approaches and show the performances of the corresponding preconditioners

A weighted global GMRES method with deflation for solving linear Sylvester equations吴钢¹³⁰

Abstract: We propose a weighted global GMRES method with deflation for solving large and spares Sylvester matrix equations. We first consider how to choose the weighting matrix during cycles, and focus on solving the weighted harmonic Ritz pairs in the weighted global Arnoldi process. Then, we knit the deflation strategy with the weighted global GMRES method, and shed light on why the new strategy can speed up the computation of large and spares Sylvester matrix equations. Numerical experiments show efficiency of our new algorithms.

¹²⁹ 殷俊峰, 同济大学数学科学学院.¹³⁰ 吴钢, 中国矿业大学数学学院. Email: gangwu@cumt.edu.cn

Efficient numerical algorithms for computing positive interior transmission eigenvalues李铁香¹³¹

Abstract: We propose an efficient eigensolver for computing densely distributed spectrum of the two-dimensional transmission eigenvalue problem (TEP) which is derived from Maxwell's equations with Tellegen media and the transverse magnetic mode. The discretized governing equations by the standard piecewise linear finite element method give rise to a large-scale quadratic eigenvalue problem (QEP). Our numerical simulation shows that half of the positive eigenvalues of the QEP are densely distributed in some interval near the origin. The quadratic Jacobi-Davidson method with a so-called non-equivalence deflation technique is proposed to compute the dense spectrum of the QEP. Extensive numerical simulations show that our proposed method makes the convergence efficiently even it needs to compute more than 5000 desired eigenpairs. Numerical results also illustrate that the computed eigenvalue curves can be approximated by the nonlinear functions which can be applied to estimate the denseness of the eigenvalues for the TEP.

Analysis of a new dimension-wise splitting iteration with selective relaxation for saddle point problems牛强¹³²

Abstract: In this talk, we will discuss a new Dimension-wise Splitting with Selective Relaxation (DSSR) method for structured system of linear equations arising from the discretization of the incompressible Navier-Stokes equations. On the selection of the relaxation parameter, Fourier analysis will be adopted to determine the optimal parameter that leads to the best performance of the iterative method for the Stokes and the steady Oseen equations. We also explore numerically the influence of boundary conditions on the optimal choice of the parameter. The use of inner and outer iterations will also be evaluated on a lid driven cavity flow.

¹³¹ 李铁香, 东南大学数学学院. Email: txli@seu.edu.cn

¹³² 牛强, 西交利物浦大学数学科学系. Email: qiang.niu@xjtlu.edu.cn

A new iterative method for solving complex symmetric linear systems

张建华¹³³

Abstract: Based on implementation of the quasi-minimal residual (QMR) and biconjugate A-orthogonal residual (BiCOR) method, in this talk, a new Krylov subspace method is presented for solving complex symmetric linear systems. The new method can be combined with arbitrary symmetric preconditioners. The preconditioned modified Hermitian and Skew-Hermitian splitting (PMHSS) preconditioner is used to accelerate the convergence rate of this method. Numerical experiments indicate that the proposed method and its preconditioned version are efficient and robust, in comparison with other Krylov subspace methods.

Inner-outer iterative variants of the CMRH method for solving multi-shifted non-Hermitian linear systems

顾先明¹³⁴

Abstract: The multi-shifted linear systems with non-Hermitian matrices often arise from the numerical solutions for time-dependent partial/fractional differential equations (PDEs/FDEs), control theory, PageRank problem, etc. In the present talk, we derive the variants of restarted CMRH (Changing Minimal Residual method based on the Hessenberg process), in which the Hessenberg process is always cheaper than the conventional Arnoldi procedure, for solving such sequence of shifted linear systems. In order to accelerate the iterative solvers, we also present both methods inside of a general framework which allows these techniques to be extended to the setting of flexible preconditioning and inexact Krylov subspace methods. Finally, extensive numerical experiments involving the numerical solutions of PDEs/FDEs and PageRank problems are reported to illustrate the performance of these proposed methods, also against other popular multi-shifted Krylov subspace methods.

¹³³张建华, 东华理工大学数学系. Email: zhangjhnuaa@163.com

¹³⁴顾先明, 电子科技大学数学科学学院. Email: guxianming@live.cn

T01-3 微分方程数值计算及应用

非平衡辐射扩散问题的渐近保持数值模拟

崔霞, 袁光伟, 沈智军¹³⁵

Abstract: 基于含有 Larsen 限流扩散算子的两温模型, 研究平几何、球对称和柱对称几何下非平衡辐射扩散问题的渐近保持离散方法。采用有限体积空间离散, 克服原点和极轴处的奇异性并保持局部守恒性。对边界处的限流算子, 采用不同于传统一阶近似的非对称二阶精度空间近似, 以确保格式具有更高阶的整体相容误差。对球几何调和平均进行了分析, 表明了其二阶精度。给出不同离散扩散算子的截断误差。利用形式分析, 证明这些格式及其结合了隐式平衡和线性化隐式时间离散的全离散格式具有一阶渐近保持性质。通过设计相关的人造解和参考解, 利用数值实验, 验证了全离散格式的良好性质, 定量地表明这些格式具有二阶精度和一阶渐近保持性质, 从而适用于平衡和非平衡辐射扩散问题数值模拟。

Computing the p-Spectral Radii of Uniform Hypergraphs with Applications

Jingya Chang, Weiyang Ding, Liquan Qi, Hong Yan¹³⁶

Abstract: The p-spectral radius of a uniform hypergraph covers many important concepts, such as Lagrangian and spectral radius of the hypergraph, and is crucial for solving spectral extremal problems of hypergraphs. In this paper, we establish a spherically constrained maximization model and propose a first-order conjugate gradient algorithm to compute the p-spectral radius of a uniform hypergraph (CSRH). By the semialgebraic nature of the adjacency tensor of a uniform hypergraph, CSRH is globally convergent and obtains the global maximizer with a high probability. When computing the spectral radius of the adjacency tensor of a uniform hypergraph, CSRH stands out among existing approaches. Furthermore, CSRH is competent to calculate the p-spectral radius of a hypergraph with millions of vertices and to approximate the Lagrangian of a hypergraph. Finally, we show that the CSRH method is capable of ranking real-world data set based on solutions generated by the p-spectral radius model.

¹³⁵ 崔霞, 北京应用物理与计算数学研究所. Email: cuixia09@163.com¹³⁶ 常静雅, 香港理工大学. Email: cxx625188@163.com

基于 BCC/FCC 晶格的金属材料微观力学行为分析

余翌帆、崔俊芝、杨彦韬¹³⁷

Abstract: Cauchy-Born 准则是在微纳米尺度物理性能计算中被广泛使用的一种变形规则，然而经典的 Cauchy-Born 准则仅仅适用于块状晶体均匀变形的情形。如果将其不加修正地运用于非均匀变形的原子体系，则会带来较大的误差。大多数晶体材料都有着规则的微观拓扑结构，其微观结构直接影响着材料的力学性质，因此直接使用微观晶格作为基本变形单元计算材料力学行为会更加符合物理本性。本文发展了修正的 Cauchy-Born 准则，对于高阶非线性变形，修正的 Cauchy-Born 准则可以更准确地表征原子体系的变形行为。同时，本文发展了基于 BCC/FCC 晶格的基本变形单元，推导了变形梯度张量 F 和应变能密度 ω ；应用上述公式，证明了具有 FCC/BCC 晶格结构的金属晶粒，在受到拉伸-压缩或者剪切变形且幅度不大时，其内部晶胞倾向于发生线性变形；进而说明晶粒变形受力变形幅度较大时，其内部晶胞会发生非线性变形，即产生了位错。

3D Simulation of the Defect Generation by Hydrogen at $Si - SiO_2$ Interface

Zhaocan Ma, Jingjie Xu, Hongliang Li, Yu Song, Linbo Zhang, Bemzhuo Lu¹³⁸

Abstract: In order to study defect generation and radiation-induced interface in semiconductor influenced by dose rate response and H_2 , we provide a 3D finite element model based on Poisson-Nernst-Planck equations to simulate the electro-diffusion process in numerical experiment. Multi-scale method is used in discretization and the restricted additive Schwarz preconditioner is applied to solve the linear system in simulation. The algorithm we establish in this work is solved by our parallel finite element software based on Parallel Hierarchical Grid with high efficiency. It is shown that the numerical results from our simulation agree well with experimental data of the devices affected by enhanced low dose-rate sensitivity in different H_2 environments.

¹³⁷ 余翌帆, 中国科学院数学与系统科学研究院. Email: yuyifan@lsec.cc.ac.cn

¹³⁸ 马召灿, 中科院计算数学所. Email: zhaocanma@lsec.cc.ac.cn

一类含奇异项的微分积分方程的适定性理论及其在稳态 Wigner 方程中的应用

朱湘疆¹³⁹

Abstract: 在量子器件的模拟中, 描述量子分布的稳态 Wigner 方程具有重要意义。然而, Wigner 方程是含奇异项的积分微分方程, 关于其解的适定性理论我们所知甚少。我们将在更一般的框架下讨论一类含奇异项的积分微分方程的适定性理论。我们将证明, 在一般的 Sobolev 空间下求解这类方程是无法奏效的。即使初值和势选取得充分理想, 方程的解仍必然出现奇异性, 使得问题无法架构在一般的 Sobolev 空间上。然而, 通过合理地对 Sobolev 空间进行“扩充”, 即添加一些具有奇异性的函数族, 我们可以严格证明在一定条件下的解的适定性。进而, 可以完全解决稳态 Wigner 方程初值问题的适定性问题。此外, 我们将针对解的形式, 设计相应的数值算法, 并给出相应的稳定性分析。

T06-3 有限元和边界元方法

The time-dependent flexural shell model and its numerical simulations

沈晓芹, 李昊明, 高志明, 秦新强¹⁴⁰

Abstract: The theory of elastic shells is one of the most important branches of the theory of elasticity. Among all the shell models, a classical and widely recognized model is the Koiter model. Under specific geometric assumptions, spatial assumptions and various boundary conditions, Ciarlet and his colleagues further classified the shell models into the membrane shell model and the flexural shell. In this talk, we discuss the time-dependent flexural model, which has not been addressed numerically. We show that the solution of the time-dependent flexural model exists and is unique. We semi-discretize the space variables and fully discretize the problems using the time discretization by the Newmark scheme. The corresponding analyses of existence, uniqueness, stability, convergence and a priori error estimate are given. Finally, we provide numerical experiments with a portion of the cylindrical shell and a portion of the conical shell to demonstrate the efficiency of the time-dependent flexural model.

¹³⁹朱湘疆, 北京大学. Email: zxj709@pku.edu.cn

¹⁴⁰沈晓芹, 西安理工大学. Email: xqshen@xaut.edu.cn

A Partially Penalized Immersed Interface Finite Element Method for Planar Elasticity Interface Problems

Peiqi Huang(NJFU), Zhilin Li(NCSU)¹⁴¹

Abstract: In this article, we have proposed a partially penalized immersed interface finite element method both in triangular and rectangular triangulations. The discrete form is proved to be stable assuming the penalty parameter is sufficiently large. The error estimates are derived to be optimal both in energy norm and L^2 norm. At last, numerical experiments are presented to confirm the theoretical results.

A Weak Galerkin Method with an Over-Relaxed Stabilization for Low Regularity Elliptic Problems

Lunji Song, Kaifang Liu, Shan Zhao¹⁴²

Abstract: A new weak Galerkin (WG) finite element method is developed and analyzed for solving second order elliptic problems with low regularity solutions in the Sobolev space $W^{2,p}(\Omega)$ with $p \in (1, 2)$. A WG stabilizer was introduced by Wang and Ye (Math Comput 83:2101–2126, 2014) for a simpler variational formulation, and it has been commonly used since then in the WG literature. In this work, for the purpose of dealing with low regularity solutions, we propose to generalize the stabilizer of Wang and Ye by introducing a positive relaxation index to the mesh size h . The relaxed stabilization gives rise to a considerable flexibility in treating weak continuity along the interior element edges. When the norm index $p \in (1, 2)$, we strictly derive that the WG error in energy norm has an optimal convergence order $O(h^{l+1-1/p-p/4})$ by taking the relaxed factor $\beta = 1 + 2/p-p/2$, and it also has an optimal convergence order $O(h^{l+2-2/p})$ in L^2 norm when the solution $u \in W^{l+1,p}$ with $p \in [1, 1 + 2/p-p/2]$ and $l \geq 1$. It is recovered for $p = 2$ that with the choice of $\beta = 1$, error estimates in the energy and L^2 norms are optimal for the source term in the sobolev space L^2 . Weak variational forms of the WG method give rise to desirable flexibility in enforcing boundary conditions and can be easily implemented without requiring a sufficiently large penalty factor as in the usual discontinuous Galerkin methods. In addition, numerical results illustrate that the proposed WG method with an over-relaxed factor $\beta(\geq 1)$ converges at optimal algebraic rates for several low regularity elliptic problems.

¹⁴¹黄佩奇, 南京林业大学. Email: pqhuang@njfu.edu.cn

¹⁴²宋伦继, 兰州大学. Email: song@lzu.edu.cn

Nonconforming virtual element method for plate bending problems

赵纪坤, 陈绍春, 张蓓¹⁴³

Abstract: We develop the nonconforming virtual element method for linear plate bending problems. A class of nonconforming virtual elements is constructed, which is C^0 -continuous. Like the classical nonconforming plate elements, it relaxes the continuity requirement for the function space to some extent. Further, the virtual element is constructed for any order of accuracy and adapts to complicate element geometries. We present a general framework on the error analysis for the nonconforming virtual element method, highlighting the main difference with the conforming one.

Error estimate of CGDG method and its fast evaluation for Maxwell's equations in Cole-Cole dispersive media

Jiangxing Wang, Jiwei Zhang, Zhimin Zhang¹⁴⁴

Abstract: The study of this paper is two-fold: we first construct an approach of combining the DG method in space with CG method in time (CG-DG method) to discretize the Cole-Cole dispersive model. We analyze the L^2 -stability and error estimate in the order of $O(\tau^r + h^{k+1/2})$ for the CG-DG method, where r and k represent the degrees of polynomials for spatial and temporal discretization, respectively. Since the Cole-Cole dispersive model involves a time-fractional derivative, which requires information about all the previous layers. The computational cost and storage will be huge for a longer time simulation. This leads to the second part of our study. An efficient algorithm is constructed based on CG method in time where the time-fractional derivative is evaluated via a sum-of-exponentials approximation for the convolution kernel. The resulting fast algorithm reduces the computational cost and storage from $O(rMN^2)$ and $O(rMN)$ for the direct method above to $O(rMN\log^2(N))$ and $O(rM\log^2(N))$, where M is the total number of unknown freedoms in space, N is the total number of time steps. Numerical examples are given to demonstrate the performance of the proposed numerical methods.

¹⁴³ 赵纪坤, 郑州大学. Email: jkzhao@zzu.edu.cn

¹⁴⁴ 王疆兴, 北京计算科学研究中心. Email: jxwang@csrc.ac.cn

Enzyme and Nanopore Simulations by Finite Element Method

许竞劼, 谢妍, 卢本卓¹⁴⁵

Abstract: The Poisson-Nernst-Planck equations are widely used in simulating the electro-diffusion processes for nanoscale biological system. Here, we apply the Poisson-Nernst-Planck equations to acetylcholinesterase system as well as nanopore and solve the equations with finite element method. We compare the numerical results of substrate-enzyme system with Debye-Hückel limiting law, which based on a linearized Poisson-Boltzmann model and known for its accurate predictions in dilute solutions. It is observed that both charged substrate and product together contribute like a non-reactive species in numerical simulation, and our Poisson-Nernst-Planck model recovers the Debye-Hückel limiting law well. For nanopore, we observe the ion current rectification phenomenon in steady state, which is influenced by nanopore geometry, electrolyte concentration and surface charge density. Moreover, nanopore scanning is simulated by time-dependent Poisson-Nernst-Planck equations, and the profile of current-voltage behavior is presented.

¹⁴⁵许竞劼, 中国科学院数学与系统科学研究院. Email: 404459611@qq.com

T07-1 多重网格技术、区域分解及并行计算

An efficient parallel iteration algorithm for radiation diffusion equationYao Yanzhong¹⁴⁶

Abstract: The radiation hydrodynamic problem is a classic multi-physical and multi-scale problem, which occurs in many applications such as inertial confinement fusion (ICF), strong explosion and astrophysical systems. When we numerically simulate this problem, we usually need to solve the radiation diffusion equations with discontinues or multi-scale coefficients. Owing to the numerical stability, we use the fully implicit computation scheme to discretize these equations, which lead to a large nonlinear algebraic system at each time step. The computational cost of solving this system is very expensive, and so we have to use massive parallel computer in order to get the numerical solution within an acceptable time. However the implicit scheme cannot be implemented directly on parallel computer since there is strong data coupling among the computation meshes, it is very difficult to design the parallel computation method. In this talk, we discuss an efficient parallelization algorithm for the radiation diffusion equation. This algorithm is based on the domain decomposition method, and it integrates the extrapolation technique and the Jacobi style semi-implicit scheme, which present a novel prediction approach for the inner bound values of the sub-domains. This algorithm makes the prediction value of the inner bound more reasonable and gives relatively accurate iterative initial value, which can decrease the number of iterations and improve the parallel computation efficiency remarkably.

Superconvergence two-grid scheme based on shifted-inverse power method for eigenvalue problems by function value recoveryLiu Huipo¹⁴⁷

Abstract: In the paper, an improved two-grid scheme based on shifted-inverse power method is pro-posed to solve the elliptic eigenvalue problems. With this new scheme, the solution of the elliptic eigenvalue problem on a fine grid Th his reduced to the solution of the elliptic eigenvalue problem and the recovered eigenfunction on a much coarser grid TH , and the solution of a elliptic bound-ary value problem and the recovered solution on the fine grid Th . Theoretical analysis shows that the scheme allow a much coarser mesh to achieve the superconvergence rate. Finally, some numerical experiments are carried out to confirm the theoretical analysis.

¹⁴⁶姚彦忠, 北京应用物理与计算数学研究所. Email: yao_yanzhong@iapcm.ac.cn¹⁴⁷刘会坡, 北京应用物理与计算数学研究所. Email: liuhuipo@amss.ac.cn

Substructuring Preconditioners with a Simple Coarse Space for 2-D 3-T Radiation Diffusion Equations

Xiaoqiang Yue, Shi Shu, Junxian Wang and Zhiyang Zhou¹⁴⁸

Abstract: Inspired by [Q. Y. Hu, S. Shu and J. X. Wang, Math. Comput., 79 (272) (2010): 2059-2078], we firstly present two nonoverlapping domain decomposition (DD) preconditioners B_h^a and B_h^{sm} about the preserving-symmetry finite volume element (SFVE) scheme for solving two-dimensional three-temperature radiation diffusion equations with strongly discontinuous coefficients. It's worth mentioning that both B_h^a and B_h^{sm} involve a SFVE sub-system with respect to a simple coarse space and SFVE sub-systems which are self-similar to the original SFVE system but embarrassingly parallel. Next, the nearly optimal estimation $\mathcal{O}((1 + \log \frac{d}{h})^3)$ on condition numbers is proved for the resulting preconditioned systems, where d and h respectively denote the maximum diameters in coarse and fine grids. Moreover, we present algebraic and parallel implementations of B_h^a and B_h^{sm} , develop parallel PCG solvers, and provide the numerical results validating the aforementioned theoretical estimations and stating the good algorithmic and parallel scalability.

并行求解平面波 Helmholtz 和 Maxwell 离散系统

袁龙, 胡齐芽, 安恒斌¹⁴⁹

Abstract: 在之前的工作中, 我们提出利用一类非重叠区域分解预条件子求解 Helmholtz 和 Maxwell 方程组的平面波离散系统。本文我们提出了该预条件子的重叠版本, 并给出了它们的效能比较。本文的主要目标是阐述预条件子的并行实现。

A Parallel Multigrid Method For Semilinear Elliptic Equation

徐飞¹⁵⁰

Abstract: A kind of multigrid finite element method is proposed for semilinear elliptic equations. The main idea is to transform the solution of the semilinear problem into a series of solutions of the corresponding linear boundary value problems on the sequence of finite element spaces and semilinear problems on a very low dimensional space. The linearized boundary value problems are solved by some multigrid iterations. The optimality of the computational work is also proved. Compared with the existing multigrid methods which need the bounded second order derivatives of the nonlinear term, the proposed method only needs the bounded first order derivative of the nonlinear term. Besides, this method has a good scalability by the parallel computing skill.

¹⁴⁸ 岳孝强, 湘潭大学. Email: yuxq@xtu.edu.cn

¹⁴⁹ 袁龙, 山东科技大学. Email: yuanlong@lsec.cc.ac.cn

¹⁵⁰ 徐飞, 北京工业大学. Email: xufei@lsec.cc.ac.cn

Multigrid Methods for A Mixed Finite Element Method of The Darcy-Forchheimer Model

Jian Huang¹⁵¹

Abstract: An efficient nonlinear multigrid method for a mixed finite element method of the Darcy-Forchheimer model is constructed in this paper. A Peaceman-Rachford type iteration is used as a smoother to decouple the nonlinearity from the divergence constraint. The nonlinear equation can be solved element-wise with a closed formulae. The linear saddle point system for the constraint is reduced into a symmetric positive definite system of Poisson type. Furthermore an empirical choice of the parameter used in the splitting is proposed and the resulting multigrid method is robust to the so-called Forchheimer number which controls the strength of the nonlinearity. By comparing the number of iterations and CPU time of different solvers in several numerical experiments, our multigrid method is shown to convergent with a rate independent of the mesh size and the Forchheimer number and with a nearly linear computational cost.

Convergence Analysis and Numerical Implementation of a Second Order Numerical Scheme for the Three-Dimensional Phase Field Crystal Equation

Lixiu Dong¹⁵²

Abstract: I will talk about the analyze and implement a second-order-in-time numerical scheme for the three-dimensional phase field crystal (PFC) equation. The PFC equation is a high-order (sixth-order) nonlinear partial differential equation. The second order numerical scheme is based on convex splitting, with the unique solvability and unconditional energy stability established. However, its convergence analysis remains open. I will present a convergence analysis, in which maximum norm estimate of the numerical solution plays an essential role. Moreover, I will outline the detailed multigrid method to solve the highly nonlinear numerical scheme over a cubic domain, and various three-dimensional numerical results are presented, including the numerical convergence test, complexity test of the multigrid solver and the polycrystal growth simulation.

¹⁵¹黄健, 山东大学. Email: yghuangjian@sina.com

¹⁵²董丽秀, 北京师范大学. Email: lixdong@mail.bnu.edu.cn

T09-3 分数阶方程

Implicit-Explicit difference schemes for nonlinear fractional differential equations with smooth inputs曹婉容, 曾凡海, 张中强, George Karniadakis¹⁵³

Abstract: We propose second-order implicit-explicit (IMEX) time-stepping schemes for nonlinear fractional differential equations with fractional order $0 < \beta < 1$. From the known structure of the non-smooth solution and by introducing corresponding correction terms, we can obtain uniformly second-order accuracy from these schemes. We prove the convergence and linear stability of the proposed schemes. Numerical examples illustrate the flexibility and efficiency of the IMEX schemes and show that they are effective for nonlinear and multi-rate fractional differential systems as well as multi-term fractional differential systems with non-smooth solutions.

Simultaneous inversion of the fractional order and the space-dependent source term for the time-fractional diffusion equation阮周生¹⁵⁴

Abstract: In this paper a simultaneous identification problem of the spacewise source term and the fractional order for a time fractional diffusion equation is considered. Firstly, the regularized properties of the solution to the direct problem is derivated. Then under some assumption and with two different kinds of observation datas for one-dimensional and two-dimensional time fractional diffusion equation, the unique results of the inverse problem are proven by the laplace transformation method and analytic continuation technique. Furthermore the inverse problems are transformed into Tikhonov type optimization problems, the existence of the optimal solutions to the Tikhonov functional is proven. At last, we construct an alternation iteration inversion method to solve the optimization problems. The efficiency and stability of the proposed method are tested by several one- and two-dimensional examples.

¹⁵³ 曹婉容, 东南大学. Email: wanrongcao@gmail.com¹⁵⁴ 阮周生, 东华理工大学. Email: zhshruan@sina.com.cn

High-order BDF convolution quadrature for fractional evolution equations

Bangti Jin, Buyang Li, Zhi Zhou¹⁵⁵

Abstract: We develop proper correction formulas at the starting $k-1$ steps to restore the desired k th-order convergence rate of the k -step BDF convolution quadrature for discretizing evolution equations involving a fractional-order derivative in time. The desired k th-order convergence rate can be achieved even if the source term is not compatible with the initial data, which is allowed to be nonsmooth. Extensive numerical examples are provided to illustrate the effectiveness of the proposed scheme.

Quantitative dependence analysis on the horizon for nonlocal diffusion models

Qiang Du, Xuying Zhao¹⁵⁶

Abstract: In this talk, several decomposition properties for nonlocal norms of double integrals arising from nonlocal models will be presented. Based on it, how the equivalence between the energy norm and the Sobolev space norm depends on the horizon and other parameters for nonlocal diffusion models will be revealed. More results with quantitative dependence on the horizon and other parameters are further established, such as the nonlocal Poincaré inequality, the priori error estimation, and condition numbers of the stiffness matrix and preconditioned stiffness matrix by diagonal scaling on quasi-uniform meshes. Both the case of integrable kernels and the case of non-integrable kernels are considered herein.

时间分数阶扩散方程高精度数值格式的修正

金邦梯, 李步扬, 周知¹⁵⁷

Abstract: In this talk, I will discuss some effective high-order numerical schemes for evolution equations involving a fractional-order derivative in time, which have been widely used to simulate the anomalous diffusion dynamics. We develop proper correction formulas at the starting $k-1$ steps to restore the desired k th-order convergence rate of the k -step BDF convolution quadrature. The desired k th-order convergence rate can be achieved even if the source term is not compatible with the initial data, which is allowed to be non-smooth. Numerical experiments support the theoretical findings.

¹⁵⁵ 李步扬, The Hong Kong Polytechnic University. Email: libuyang@gmail.com

¹⁵⁶ 赵旭鹰, 中科院数学与系统科学研究院. Email: zhaoxy@lsec.cc.ac.cn

¹⁵⁷ 周知, 香港理工大学. Email: zhouzhi19880125@gmail.com

Asymptotic behaviours and numerical approximations for F-ODEs and F-FDEs

Dongling Wang, Northwest University.¹⁵⁸

Abstract: We first provide some new asymptotic behaviors of F-ODEs and F-FDEs. Then we study the dissipativity of F-ODEs and F-FDEs with a bounded absorbing set, and the asymptotic stability and the contractivity of F-ODEs and F-FDEs with algebraically decay rate. Some numerical schemes are further constructed for F-ODEs and F-FDEs. These schemes are proved to be dissipative and contractive, and can preserve the exact decay rate as the continuous equations. Several numerical examples are given to illustrate the advantages of the structure-preserving numerical methods.

分会场报告 4

S01-2 PDE 并行、快速算法研究进展

A parallel finite element method for 3D moving contact line problem in complex domain with applications

罗力¹⁵⁹

Abstract: Moving contact line problem plays an important role in fluid-fluid interface motion on solid surfaces. The problem can be described by a phase-field model consisting of the coupled Cahn-Hilliard and Navier-Stokes equations with the generalized Navier boundary condition (GNBC). We generalize the GNBC to surfaces with complex geometry and introduce a finite element method on unstructured 3D meshes. Accurate simulation of the interface and contact line motion requires very fine meshes, and the computation in 3D is even more challenging. Thus, the use of high performance computers and scalable parallel algorithms are indispensable. A highly parallel solution strategy using different solvers for different components of the discretization is presented. Parallel performances show that the strategy is scalable for 3D problems on a supercomputer with a large number of processors. We apply the proposed schemes and solution algorithms to study several important applications, particularly for those phenomena that can not be achieved by 2D simulations.

¹⁵⁸ 王冬岭, 西北大学. Email: wdymath@nwu.edu.cn

¹⁵⁹ 罗力, 中国科学院深圳先进技术研究院. Email: li.luo@siat.ac.cn

A divergence free virtual element method for the Stokes problem on polyhedral meshes

王锋¹⁶⁰

Abstract: In this talk, we shall propose some virtual element methods on polygonal and polyhedral meshes for the Stokes problem. The pressure is approximated by discontinuous polynomials, while the velocity is discretized by $H(\text{div})$ virtual elements with some tangential polynomials on the faces. The main feature of the method is that it preserves the divergence free constraint exactly, and therefore the error estimates for the velocity does not explicitly depend on the pressure.

A Domain Decomposition Based Method for the Simulation of Wind Flows over Large Urban Areas

闫争争¹⁶¹

Abstract: Accurate prediction of the wind flow field in large urban areas is the basis of many applications such as the vulnerability analysis of tall buildings and air pollution forecast. In this talk, we present a scalable domain decomposition based method for the numerical simulation of flows in urban areas with detailed geometric information of buildings. Two approaches are investigated including a 3D incompressible Navier-Stokes model and a LES with the Smagorinsky subgrid model. We report the parallel performance of the algorithm on supercomputers with a large number of processor cores.

Introduction of some space-time Schwarz algorithms for parabolic equation

李世顺¹⁶²

Abstract: In this talk, we introduce some two-level and multilevel space-time Schwarz methods for solving linear systems arising from numerical discretization of parabolic equations. With these methods, the parabolic equations are solved parallel in both space and time directions. We develop a convergence theory and show how the convergence rate depends on the mesh sizes, the number of subdomains, and the window size. Some numerical experiments are carried out on a supercomputer computer with thousands of processors to confirm the theory in terms of the optimality and scalability.

¹⁶⁰ 王锋, 南京师范大学. Email: fengwang@live.cn

¹⁶¹ 闫争争, 中国科学院深圳先进技术研究院. Email: zhengzh.yan@gmail.com

¹⁶² 李世顺, 河南理工大学. Email: lss6@sina.com

S03-2 界面问题的建模与计算

A Cartesian grid method for moving interface problems应文俊¹⁶³

Abstract: In this talk, I will present a Cartesian grid method for moving interface problems. The method represents a moving interface, curve in 2D and surface in 3D, by its intersection with an underlying Cartesian grid. This representation not only avoids generation of unstructured interface triangulation but also makes it convenient to compute geometry properties of the interface. When evaluation of a boundary integral is needed, the representation also naturally provides a super-algebraic convergent numerical quadrature. Numerical examples for mean curvature flows and two-phase Stokes flows will be presented.

A parametric finite element method for solid-state dewetting problems with anisotropic surface energies蒋维¹⁶⁴

Abstract: We propose an efficient and accurate parametric finite element method (PFEM) for solving sharp-interface continuum models for solid-state dewetting of thin films with anisotropic surface energies. The governing equations of the sharp-interface models belong to a new type of high-order (4th- or 6th-order) geometric evolution partial differential equations about open curve/surface interface tracking problems which include anisotropic surface diffusion flow and contact line migration. Compared to the traditional methods (e.g., marker-particle methods), the proposed PFEM not only has very good accuracy, but also poses very mild restrictions on the numerical stability, and thus it has significant advantages for solving this type of open curve evolution problems with applications in the simulation of solid-state dewetting. Extensive numerical results are reported to demonstrate the accuracy and high efficiency of the proposed PFEM.

自由表面问题的混合元方法及其快速算子

王何宇¹⁶⁵

Abstract: 文章讨论了针对自由表面问题的 2D 和 3D 混合元 NS 方程求解算法, 以及相应的无结构多重网格预处理快速求解算子的构建。在实现多重网格效率的同时, 数值结果和物理实验以及 thin film 模型的计算结果进行了比较。

¹⁶³ 应文俊, 上海交通大学. Email: wying@sjtu.edu.cn¹⁶⁴ 蒋维, 武汉大学. Email: jiangwei1007@whu.edu.cn¹⁶⁵ 王何宇, 浙江大学. Email: wangheyu@zju.edu.cn

Use Onsager Principle as an approximation tool in some liquid problems with moving interfaces

许现民¹⁶⁶

Abstract: In this talk, we will present several examples using Onsager principle as an approximation tool in moving interface problems. They are sliding liquids on a substrate, a capillary rising problem of a thin liquid film, and velocity dependence of contact angle hysteresis. All these problems have moving contact lines, that are difficult to handle by standard models and computational methods. The examples show some advantages and drawbacks of the new approximation method for dynamic problems in physics. This is based on a joint work with Yana Di and Masao Doi.

S04-2 材料科学的可计算建模与计算方法

Poission-Nernst-Planck 方程的两网格有限元计算

阳莺¹⁶⁷

Abstract: Poission-Nernst-Planck (PNP) 方程是一类非线性奇性的耦合方程组，在分子静点势、离子通道和半导体领域广泛应用。利用有限元计算在求解 PNP 方程时容易出现耦合迭代发散的现象。为此，我们设计了能够对 PNP 方程解耦的两网格有限元方法。该方法的计算效率比经典的有限元方法高，并且避免了有限元方法的耦合迭代发散的现象，但仍保持有限元方法的收敛精度。我们将介绍相关的理论分析和数值计算结果。

一种求解特征值和奇异值的新型分布式并行算法

李胜国¹⁶⁸

Abstract: 在面向超级计算机时，算法的可扩展往往成为性能的瓶颈。本报告将介绍一种基于谱分而治之的新型奇异值和特征值算法，具有良好的并行可扩展性，可实现多层并行。虽然该类算法需要额外的计算量，但在利用更多计算资源后，性能却可明显地优于已有的通用算法。

¹⁶⁶ 许现民, 中国科学院数学与系统科学研究院. Email: xmxu@lsec.cc.ac.cn

¹⁶⁷ 阳莺, 桂林电子科技大学. Email: yangying@lsec.cc.ac.cn

¹⁶⁸ 李胜国, 国防科学技术大学. Email: shengguols@126.com

基于平面波离散的并行轨道更新方法新进展

潘妍¹⁶⁹

Abstract: 由于并行轨道更新算法在实空间方法中的良好表现, 我们针对电子结构计算问题提出了一种基于平面波离散的并行轨道更新方法, 用于求解相应的特征值问题。此外, 我们还提出了两个新的修正并行轨道更新方法。与传统平面波方法相比, 我们的方法最大特点是两层并行。正因为两层并行的特点, 从而使得我们的方法在大规模计算中更有竞争力。数值实验表明, 在现代的超级计算机上, 对于大规模的问题这些新方法更可靠和高效。

电子结构计算的保正交共轭梯度法

张力维¹⁷⁰

Abstract: 本报告将介绍一种计算电子结构的保正交共轭梯度法。有别于传统的共轭梯度法, 我们提出一种基于 Hesse 算子的步长策略以代替在电子结构计算中难以实现的精确线搜索, 并将这一策略与三种保正交策略相结合, 得到了计算原子及分子系统基态能量的算法。在一些合理的假设下, 我们证明了该共轭梯度法的局部收敛性。同时, 我们的数值实验也表明该共轭梯度法十分高效。

The preconditioning function for the linearized DFT eigenvalue problem with plane wave basis

高兴誉¹⁷¹

Abstract: The preconditioning function proposed by Teter, Payne, and Allan plays a significant role in solving the linearized Kohn-Sham eigenvalue problem in DFT calculations. We propose a more general formula that can readily generate a class of preconditioning functions. These functions have higher order approximation accuracy and fulfill the two essential preconditioning purposes as required in plane wave DFT calculations.

¹⁶⁹ 潘妍, 中国科学院数学与系统科学研究院. Email: yanpan@lsec.cc.ac.cn

¹⁷⁰ 张力维, 中国科学院数学与系统科学研究院. Email: zhanglw@lsec.cc.ac.cn

¹⁷¹ 高兴誉, 北京应用物理与计算数学研究所.

S05-2 Recent advances in nonstandard discretization methods in scientific and engineering computation

非协调有限元特征值问题的多重网格算法

谢和虎¹⁷²

Abstract: 针对特征值问题采用非协调有限元方法进行离散, 然后设计出一种适合非协调有限元方法的多重校正算法和相应的多重网格算法, 同时给出相应的误差分析。这种多重校正算法可以提高非协调有限元特征值问题的求解效率。

Regularity for time fractional wave problems

谢小平¹⁷³

Abstract: Using the Galerkin method, we obtain the unique existence of the weak solution to a time fractional wave problem, and establish some regularity estimates which reveal the singularity structure of the weak solution in time.

Maximum principles for P1-P0 weak Galerkin finite element approximations of quasi-linear Second order elliptic equations

张然¹⁷⁴

Abstract: This talk will introduce maximum principles for the weak Galerkin method dealing with the second order elliptic equation. Under the h-acute assumption for the mesh partition, two maximum principles with respect to midpoints are proved. The theoretical analysis is based on the variational form and De Giorgi technique. Some numerical results are also presented.

The optimal EDG methods and fast solvers for the general diffusion problems

张世全¹⁷⁵

Abstract: In this talk, we first construct and analyze the optimal EDG methods for the general diffusion problems on arbitrary polygons in 2D and tetrahedra in 3D. The polynomial of degree $k+1$, $k+1$, k for potential, numerical traces and flux are provided and the optimal convergence order are derived. Then the corresponding fast solvers are constructed to solve the obtained linear systems. The obtained solvers can also be applied to a general range of elements, include the arbitrary order conforming elements on triangles and quadrilaterals.

¹⁷²谢和虎, 中国科学院计算数学研究所.

¹⁷³谢小平, 四川大学. Email: xpxie@scu.edu.cn

¹⁷⁴张然, 吉林大学. Email: zhangran@jlu.edu.cn

¹⁷⁵张世全, 四川大学.

Order reduced methods for fourth order problems

张硕¹⁷⁶

Abstract: Institute of Computational Mathematics, Chinese Academy of Sciences Abstract: Many model problems in applied sciences are in the formulation of fourth order problems. Their discretizations have been drawing wide interests. In this talk, some recent progress on designing and implementing order reduced methods for fourth order problems by the speaker and his collaborators will be presented. First of all, a routine framework will be given which transforms the primal fourth order problem to a stable system on a series of low order spaces. The well-posedness of the generated system and the equivalence between the primal formulation and the order reduced formulation can be guaranteed provided mild hypotheses. This way, the framework works for a wide class of fourth order problems. The new formulation admits discretisation with low-regularity finite element spaces, and convenience may thus be expected. Then, some examples are given to illustrate the implementation of the framework. A series of examples on the low-regularity discretisation of boundary value problems about several typical fourth order operators are discussed, finite element schemes are constructed for each of them, and optimal convergence rates are obtained. A second series of examples are on fourth order eigenvalue problems. With the low-regularity finite element spaces utilised, nested discretizations can be admitted. We will focus on, beyond the schemes themselves, the designing and implementation of associated multilevel method and their optimal efficiency. Examples include linear and nonlinear, and self-adjoint and non-self-adjoint problems. Some related topics can also be mentioned.

S08-3 无界域数学物理方程的数值方法及其应用

FEM and CIP-FEM for Helmholtz Equation with High Wave Number and PML truncation

武海军¹⁷⁷

Abstract: The inf-sup constant for the Helmholtz equation with high wave number and PML truncation is proved to be of order $O(1/k)$. As an application, preasymptotic error estimates for the linear FEM and CIP-FEM are derived.

¹⁷⁶张硕, 中国科学院计算数学研究所. Email: szhang@lsec.cc.ac.cn

¹⁷⁷武海军, 南京大学数学系. Email: hjw.nju@icloud.com

Boundary integral equation methods for acoustic and elastic waves

徐立伟¹⁷⁸

Abstract: In this talk, we discuss boundary integral equation methods for solving the two-dimensional fluid-solid scattering problem and the exterior elastic scattering problem. Existence and uniqueness results for variational solutions of boundary integral equations are established. Since in all these boundary variational formulations, the hypersingular boundary integral operator associated with the time-harmonic Navier equation is a dominated integral operator, we also include a new regularization formulation for this hypersingular operator, which allows us to treat the hypersingular kernel by a weakly singular kernel. A new computational approach is employed based on the series expansions of Hankel functions for the computation of weakly-singular boundary integral operators during the reduction of corresponding Galerkin equations into discrete linear systems. Numerical examples are presented to verify and validate the theoretical results.

An efficient adaptive rescaling scheme for computing moving interface problems

应文俊¹⁷⁹

Abstract: In this talk, I will present an adaptive rescaling scheme for computing long-time dynamics of expanding interfaces. The main idea is to rescale the temporal and spatial variables so that the interfaces evolve logarithmically fast at early growth stage and exponentially fast at later times. The new scales guarantee the conservation of the area/volume enclosed by the interface. Numerical examples will be presented. This is joint work with Meng Zhao, Shuwang Li and John Lowengrub.

无界域空间半离散波动方程的人工边界条件及稳定性分析

张磊¹⁸⁰

Abstract: 空间半离散的波动方程是数值模拟中一类重要的 ODE 系统，它在数值计算中有着很重要的应用，例如弹簧谐振子结构运动的模拟、线性化的一维原子链的计算等等。而在数值计算中，难点在于如何设立正确的人工边界条件以代替真实物理实际中无界区域的计算，这一方面，已经有了许多优秀的工作，如完全匹配层方法、变分边界条件、匹配边界条件等等。但是，这些方法往往都缺少了完整的稳定性分析，而这在数值模拟中是很重要的一方面。我们的工作是基于推导出的一维半无界区域的精确边界条件，通过近似处理从而得到数值计算所需的人工边界条件，并证明了一定条件下整个系统的稳定性。之后，我们还把半离散的波动方程推广到更一般的形式，以解决实际中更复杂的情形。

¹⁷⁸ 徐立伟, 电子科技大学数学学院. Email: xul@uestc.edu.cn

¹⁷⁹ 应文俊, 上海交通大学自然科学研究院. Email: wying@sjtu.edu.cn

¹⁸⁰ 张磊, 北京大学工学院. Email: zhanglei2012@pku.edu.cn

Perfectly matched layer method for electromagnetic scattering problems in layered media

郑伟英¹⁸¹

Abstract: This talk is to study the convergence of the perfectly matched layer (PML) method for electro- magnetic scattering problems in layered media. The PML method is widely used in the engineering literature and very efficient to solve wave scattering problems. In 2010, Chen and Zheng first proved the exponential convergence of PML method for the Helmholtz scattering problem in a two-layered medium. Since the background materials in the upper and lower half spaces are different, the Green function of the scattering problem in layered media becomes very complicated. Their proof is very technical and depends on elaborates estimates for the Green function. In this work, we develop a new framework for the exponential convergence of the PML method and for the well-posedness of the approximate problem. The methodology is used to three-dimensional electromagnetic scattering problems in two-layer media.

T02-3 流体力学中的数值计算

复杂构型流动问题的多介质 ALE 模拟

曾清红¹⁸²

Abstract: 在武器物理和惯性约束聚变领域，实际问题的构型非常复杂。这类问题有两个重要的特点：一是存在多种物质，物质之间由物质界面分割开；二是随着时间的演化，流场的变形很大。由于自身流场的复杂性和多物质界面的严重扭曲，这种多介质大变形问题在理论研究中存在诸多难点，具有很强的挑战性，目前数值模拟是其重要的研究手段之一。本文基于多介质任意拉格朗日-欧拉框架（Multi-Material Arbitrary Lagrangian Eulerian, MMALE），在传统 ALE 方法基础上引入混合网格，允许计算网格边界跨过物质界面，采用 MOF 方法（Moment of Fluid）进行界面重构，应用于复杂构型流动问题的数值模拟研究。数值算例表明，多介质 ALE 方法是模拟复杂构型流动问题的有效手段，具有较好的数值精度和界面分辨率，并且具有较好的健壮性。

¹⁸¹ 郑伟英, 中国科学院数学与系统科学研究院. Email: zwy@lsec.cc.ac.cn

¹⁸² 曾清红, 北京应用物理与计算数学研究所. Email: qinghzeng@qq.com

健壮的流体力学一维形式黎曼解

沈智军¹⁸³

Abstract: 多介质大变形问题的数值模拟，是辐射流体力学问题数值模拟中最具挑战性的课题之一。模拟这类问题，往往采用能够精确分辨物质界面的拉格朗日方法或者其修正版：任意欧拉拉格朗日方法（ALE 方法）。建立在局部一维黎曼解为基础的 Godunov 数值方法在模拟多介质大变形问题时，特别是在模拟强激波问题时，容易出现一些非物理现象，如伪涡度误差和数值激波不稳定现象。这些不稳定现象常常导致计算结果的失准甚至计算过程的中断。该类缺陷源于传统数值方法自身的设计方式，因此仅靠加密计算网格，减少时间步长，采用高精度技术等传统方法并不能改正这些缺点。针对数值方法中存在的问题，我们提出了一种新的二维稳定性分析方法，并进一步提出了一种基于拉格朗日方法的涡度分析方法，寻找到了造成网格扭曲的格式原因。同时设计了适用于无结构网格上激波计算的健壮的数值方法。该方法可以清晰分辨物质界面，可以有效地克服传统数值格式存在的数值激波不稳定性等多种非物理现象。目前，该方法已被应用到欧氏、拉氏及 ALE 方法中，并取得了很好的计算效果。

流动诱导聚合物结晶的建模与模拟

王晓东¹⁸⁴

Abstract: 针对聚合物晶体形态模拟，提出了一种改进的粗颗粒化相场模型，该模型可以在静态条件下模拟预测多种晶体形态，所得结果与实验定性吻合。在此基础上，进一步考虑流动对聚合物结晶的影响。利用分子哑铃模型描述聚合物大分子取向，Navier-Stokes 方程描述粘弹流动，构型场中的取向椭圆量化流动诱导成核，改进相场模型描述晶体生长。通过以上物理场或物理过程的耦合，建立了聚合物流动与结晶共存体系的可计算模型。基于该模型，探索了流动对聚合物单晶形态及流道中晶体分布的影响规律。

¹⁸³ 沈智军, 北京应用物理与计算数学研究所. Email: shen_zhijun@iapcm.ac.cn

¹⁸⁴ 王晓东, 西北工业大学. Email: xiaodongwang@nwpu.edu.cn

Linear Energy Stable Scheme for Quasi-incompressible Hydrodynamic Binary Fluid Model

Yuezheng Gong, Jia Zhao, Qi Wang¹⁸⁵

Abstract: In this talk, we develop spatial-temporally second-order, energy stable numerical schemes for two classes of hydrodynamic phase field models of binary viscous fluid mixtures of different densities. One is quasi-incompressible in which the velocity field is the mass average velocity, while the other is incompressible in which the velocity field is volume average one. We introduce a novel linearization technique to arrive at fully discrete linear schemes, where in each time marching step only a linear algebraic equation system needs to be solved. In particular, the linearization technique does not rely on the specific form of the bulk free energy so long as it is bounded below. These schemes are then proved to be unconditionally energy stable rigorously subject to periodic boundary conditions so that a large time step is plausible. Both spatial and temporal mesh refinements are presented to illustrate the second order accuracy of the schemes. Several numerical examples, including coarsening dynamics of two immiscible fluids and a heavy fluid drop settling in a lighter fluid matrix, are presented to show the accuracy and effectiveness of our proposed linear schemes. Predictions by the two fluid mixture models are compared and discussed. As the density difference between the two fluid components are large, the two hydrodynamic phase field models indeed predict quite distinct transient dynamics. We believe the quasi-incompressible model is more reliable than the incompressible one.

Free boundary value problem to 3D spherically symmetric compressible Navier–Stokes–Poisson equations

Huihui Kong , Hai-Liang Li¹⁸⁶

Abstract: We consider the free boundary value problem to 3D spherically symmetric compressible isentropic Navier–Stokes–Poisson equations for self-gravitating gaseous stars with γ -law pressure density function for $6/5 < \gamma \leq 4/3$. For stress-free boundary condition and zero flow density continuously across the free boundary, the global existence of spherically symmetric weak solutions is shown, and the regularity and long time behavior of global solution are investigated for spherically symmetric initial data with the total mass smaller than a critical mass.

¹⁸⁵ 龚跃政, 北京计算科学研究中心. Email: gongyuezheng@csrc.ac.cn

¹⁸⁶ 孔慧慧, 北京计算科学研究中心. Email: konghuihuiking@126.com

T05-2 谱方法、数值逼近与计算几何

An efficient spectral-Galerkin approximation and error analysis for Maxwell transmission eigenvalue problems in spherical geometriesJing An, Zhimin Zhang¹⁸⁷

Abstract: We propose and analyze an efficient spectral-Galerkin approximation for the Maxwell transmission eigenvalue problem in spherical geometry. Using a vector spherical harmonic expansion, we reduce the problem to a sequence of equivalent one-dimensional TE and TM modes that can be solved individually in parallel. For the TE mode, we derive associated generalized eigenvalue problems and corresponding pole conditions. Then we introduce weighted Sobolev spaces based on the pole condition and prove error estimates for the generalized eigenvalue problem. The TM mode is a coupled system with four unknown functions, which is challenging for numerical calculation. To handle it, we design an effective algorithm using Legendre-type vector basis functions. Finally, we provide some numerical experiments to validate our theoretical results and demonstrate the efficiency of the algorithms.

Pseudospectral methods for computing the multiple solutions of the Schrodinger equation李昭祥, 劳吉, 王中庆¹⁸⁸

Abstract: In this paper, we first compute the multiple non-trivial solutions of the Schrodinger equation on a square, by using the Liapunov-Schmidt reduction and symmetry-breaking bifurcation theory, combined with Legendre pseudospectral methods. Then, starting from the non-trivial solution branches of the corresponding nonlinear problem, we further obtain the whole D_4 symmetric positive solution branch of the Schrodinger equation numerically by the continuation method and pseudo-arclength algorithm. Next, we propose the extended systems, which can detect the fold and symmetry-breaking bifurcation points on the branch of the D_4 symmetric positive solutions. We also compute the multiple positive solutions with various symmetries of the Schrodinger equation by the branch switching method based on the Liapunov-Schmidt reduction. Finally, the bifurcation diagrams are constructed, showing the symmetry/peak breaking phenomena of the Schrodinger equation. Numerical results demonstrate the effectiveness of these approaches.

¹⁸⁷ 安静, 北京计算科学研究中心. Email: aj154@163.com¹⁸⁸ 李昭祥, 上海师范大学数学系. Email: zxli@shnu.edu.cn

A MATLAB-based Fourier-Spectral Solver for Phase-Field Simulations

Fei Liu¹⁸⁹

Abstract: Numerical simulations of two-phase incompressible flows using phase-field models is an invaluable research in fluid dynamics. However, there are few publicly available codes which are usually written in C or Fortran. It is difficult to simulate the model, due to the complexity of the problem. Here, we present a compact educational software package for simulating the two-phase incompressible flows in Matlab environment. Due to high order of accuracy, spectral methods are used for spatial discretization. First-order and second-order energy stable time discretization schemes are used for 2D Allen-Cahn and Cahn-Hilliard Navier-Stokes models. For the variable density, a Boussinesq approximation is used (when the density ration is small). Amply numerical tests are carried out to exhibit high speeds and numerical stability with concise codes.

Time splitting-exponential wave integrator Fourier pseudospectral method for Schrödinger-Boussinesq system

廖锋, 张鲁明¹⁹⁰

Abstract: In this report, we formulate an efficient and accurate numerical method for approximations of the coupled Schrödinger-Boussinesq (SBq) system. The main features of our method are based on: (i) the applications of a time-splitting Fourier spectral method for Schrödinger-like equation in SBq system, (ii) the utilizations of exponential wave integrator Fourier pseudospectral for spatial derivatives in the Boussinesq-like equation in SBq system. The scheme is fully explicit and efficient due to fast Fourier transform. The numerical examples are presented to show the efficiency and accuracy of our method.

¹⁸⁹ 刘飞, 华中科技大学. Email: liufei_2000@163.com

¹⁹⁰ 廖锋, 南京航空航天大学. Email: wawjd3kwcom@163.com

Finding Excited States of Bose-Einstein Condensates by a Constrained Gentlest Ascent Dynamics

Wei Liu (Hunan Normal University)¹⁹¹

Abstract: As is known that constrained saddle points of Gross-Pitaevskii energy functionals correspond to excited states of Bose-Einstein condensates (BECs), thus in this talk, a constrained gentlest ascent dynamics (CGAD) will be proposed for stably finding these (but possibly not all) excited states which can be viewed as constrained saddle points of a Gross-Pitaevskii energy functional. First the formulation of the CGAD will be carefully designed to search a constrained saddle point with any specified index. Then an effective time-splitting strategy of CGAD based on a discrete orthonormalization process (CGAD-DON) will be presented to simplify the numerical implementation, noticing that the CGAD-DON is discretised in time by the semi-implicit backward Euler scheme and in space by the sine pseudo-spectral approximation (BESP). Finally, extensive numerical results are reported to show the efficiency of our methods, some of them are consistent with the theoretical results which are already in the literature, others show some new interesting physics but still open to be verified.

Keywords: constrained gentlest ascent dynamics, excited states, Bose-Einstein condensates, Gross-Pitaevskii energy functional, sine pseudo-spectral approximation

(Joint work with Ziqing Xie and Yongjun Yuan.)

A local-adjustment based two-dimensional Delaunay triangular mesh generation method on a bounded domain with moving boundary

Tiancheng Gao, Liyong Zhu, Hang Si¹⁹²

Abstract: In this talk, we present a two-dimensional triangular Delaunay mesh generation method based on local mesh adjustment on a bounded domain with moving boundary. By employing local mesh adjustment rather global re-generation, the developed method obtains good efficiency, while the Delaunay property of the generated mesh guarantees that the mesh has good quality. Furthermore, high dimensional embedding technology is combined with the proposed mesh generation method to generate the anisotropic mesh for a bounded domain with moving boundary. Some typical numerical examples demonstrate the effectiveness, efficiency and robust of the proposed method.

¹⁹¹ 刘伟, 湖南师范大学. Email: wliu.hunnu@foxmail.com

¹⁹² 高天成, 北京航空航天大学. Email: gtczz@sina.com

T06-4 有限元和边界元方法

非线性电磁场方程的全离散 $\mathbf{A}-\phi$ 有限元方法

姚昌辉¹⁹³

Abstract: 本文的主要内容是对非线性电磁场问题使用全离散有限元方法来做误差估计, 在时间上使用后向欧拉格式, 空间上使用节点有限元。非线性项, 是幂函数的形式, 具有单调性和连续性。我们在空间内设计一个时间离散格式, 并使用单调算子理论证明其解的适定性。通过对离散格式进行线性插值, 我们构造出等价形式, 并证明随着, 其解收敛到原变分问题的解, 进而得出时间低正则要求下的误差估计, 半离散格式的误差收敛阶; 类似的方法去处理全离散格式, 在低正则要求下得到全离散格式的误差收敛阶, 最后我们对误差估计部分加以修正使得精度提高, 这是基于较高正则假设下得到的丰满估计。在文章最后, 给出数值实验去验证我们的理论结果。

Staggered discontinuous Galerkin method for P-Stokes systems

Huang Hongying, Chung Eric¹⁹⁴

Abstract: In this paper we study the staggered discontinuous Galerkin method for systems of p-Stokes type for $p \in (1, \infty)$. We derive error estimates for approximation of the velocity and for the pressure in a suitable functional setting. The results are supported by numerical experiments.

Array-oriented Finite Element Method Programming in Python

Huayi Wei¹⁹⁵

Abstract: NumPy is the fundamental package for scientific computing with Python, which provides a powerful N-dimensional array object, sophisticated (broadcasting) functions, linear algebra and other useful functions. Based on Numpy, we introduce how to use array-oriented programming technique to reconstruct the key algorithms in finite element method. Furthermore, we introduce our new package FEALPy (Finite Element Analysis Library in Python).

¹⁹³ 姚昌辉, 郑州大学. Email: chyao@lsec.cc.ac.cn

¹⁹⁴ 黄红英, 浙江海洋大学. Email: huanghy@lsec.cc.ac.cn

¹⁹⁵ 魏华伟, 湘潭大学. Email: weihuayi@xtu.edu.cn

The effect of mesh geometry on the condition number of stiffness matrix of finite element for Plate Bending Problems

Mengying Wang, Liyong Zhu¹⁹⁶

Abstract: Abstract: It is well-known that mesh geometry affects not only the approximation error of the finite element solution but also the spectral properties of the corresponding stiffness matrix. The effect of mesh geometry of the restricted cubic Hermite finite element on the condition number of stiffness matrix is unknown for Plate Bending Problems. In this talk, we present some refined relationships between the spectral condition number of the stiffness matrix and the mesh geometry of the restricted cubic Hermite finite element defined on simplicial meshes for fourth order plate bending problems. These results provide guidance to the studies of both linear algebraic solvers and the unstructured geometric meshing.

Penalized Crouzeix-Raviart method for eigenvalue problems

马利敏¹⁹⁷

Abstract: We propose a penalized Crouzeix-Raviart element method for eigenvalue problems of second order elliptic operators. The key idea is to add a penalty term to tune the local approximation property and the global continuity property of the discrete eigenfunctions. The feature of this method is that by adjusting the penalty parameter, some of the resulted discrete eigenvalues are upper bounds of exact ones, and the others are lower bounds, and consequently a large portion of them can be reliable and approximate eigenvalues with high accuracy. Furthermore, we design an algorithm to select a penalty parameter which meets the condition. Finally we provide numerical tests to demonstrate the performance of the proposed method.

¹⁹⁶ 王梦莹, 北京航空航天大学. Email: librawmy@foxmail.com

¹⁹⁷ 马利敏, 北京大学. Email: adamalm1017@gmail.com

T09-4 分数阶方程

An analysis of the modified L1 scheme for the time-fractional partial differential equations with nonsmooth dataYubin Yan, Neville J. Ford¹⁹⁸

Abstract: We consider error estimates for the modified L1 scheme for solving time fractional partial differential equation. Jin et al. (2016, An analysis of the L1 scheme for the sub-diffusion equation with nonsmooth data, IMA J. of Numer. Anal., 36, 197-221) established an $O(k)$ convergence rate for the L1 scheme for both smooth and nonsmooth initial data. We introduce a modified L1 scheme and prove that the convergence rate is $O(k^{2-\alpha})$, $0 < \alpha < 1$ for both smooth and nonsmooth initial data. We first write the time-fractional partial differential equation as a Volterra integral equation which is then approximated by using the convolution quadratures with some special generating functions. The numerical schemes obtained in this way are equivalent to the standard L1 scheme and the modified L1 scheme, respectively. A Laplace transform method is used to prove the error estimates for the homogeneous time-fractional partial differential equation for both smooth and nonsmooth data. Numerical examples are given to show that the numerical results are consistent with the theoretical results.

Sharper error bound for a discontinuous Gakerlin, time-stepping method for a fractional stochastic diffusion equation disturbed by fraction Brownian motionsRuisheng Qi, Xiaojie Wang¹⁹⁹

Abstract: In this paper, we consider a fractional stochastic heat equation driven by infinite dimensional fractional Brownian motion with the Hurst parameter greater than one-half. We apply the piecewise constant, discontinuous Gakerlin method to discretize this equation with respect to time. By using the explicit form for the scalar resolvent function and the refined estimates for Mittag-Leffler's function, we derive sharper mean-square regularity results for the mild solution. Then based on the sharper regularity results, the sharper error bound is obtained.

¹⁹⁸ 闫玉斌, 英国切斯特大学 (吕梁学院特聘). Email: y.yan@chester.ac.uk

¹⁹⁹ 祁瑞生, 东北大学秦皇岛分校. Email: qirsh@neuq.edu.cn

A sharp maximum principle for a two-point boundary value problem with a Caputo fractional derivative

Xiangyun Meng, Martin Stynes²⁰⁰

Abstract: The analysis of finite difference methods often depends on discrete maximum principles. One can expect a difference scheme to have this property only if the boundary value problem that it approximates satisfies a continuous maximum principle. Thus it is of interest to investigate when fractional-derivative boundary value problems satisfy maximum principles—this is a non-trivial question in general. For the Caputo two-point boundary value problem that we will consider, an example shows that, unlike the classical elliptic case, Dirichlet boundary conditions won't guarantee a maximum principle. What boundary conditions will yield a maximum principle? To the best of our knowledge, only one maximum principle result is known for this Caputo problem, and it is easy to see that this result is not sharp. We derive an explicit formula for the Green's function of our boundary value problem. After some analysis of this Green's function we obtain a sharp maximum principle.

Numerical approaches to the functional distribution of anomalous diffusion with both traps and flights

Zhijiang Zhang, Weihua Deng²⁰¹

Abstract: The functional distributions of particle trajectories have wide applications. This paper focuses on providing effective computation methods for the models, which characterize the distribution of the functionals of the paths of anomalous diffusion with both traps and flights. Two kinds of discretization schemes are proposed for the time fractional substantial derivatives. The Galerkin method with interval spline scaling bases is used for the space approximation; compared with the usual finite element or spectral polynomial bases, the spline scaling bases have the advantages of keeping the Toeplitz structure of the stiffness matrix, and being easy to generate the matrix elements and to perform preconditioning. The rigorous stability analyses for both the semi and the full discrete schemes are skillfully developed. Under the assumptions of the regularity of the exact solution, the convergence of the provided schemes is also theoretically proved and numerically verified. Moreover, the theoretical background of the selected basis function and the implementation details of the algorithms involved are described in detail.

²⁰⁰ 孟祥云, 北京计算科学研究中心. Email: xymengmath@163.com

²⁰¹ 张治江, 兰州大学. Email: zhjzhang14@lzu.edu.cn

Two conservative finite element schemes for the strongly coupled nonlinear fractional Schrodinger equations

李猛, 黄乘明, 张国宇²⁰²

Abstract: This report focus on numerically solving the strongly coupled nonlinear fractional Schrodinger equations. We propose two conservative finite element schemes, containing an implicit scheme and a linearized one. We show that the schemes conserve both the mass and energy. Using the conservative properties and some Sobolev inequalities, the boundedness and convergence are established. Several numerical experiments are provided to confirm the theoretical results.

The analysis of stability and convergence of the numerical scheme for the time-fractional sub-diffusion equation with nonlocal boundary conditions

Cui-cui Ji, Zhi-zhong Sun²⁰³

Abstract: In this paper, we provide an efficient finite difference scheme for the fractional PDEs with nonlocal boundary conditions. By using the discrete energy method, we prove that the proposed scheme is unconditionally stable and convergent in maximum norm. Numerical examples support our theoretical results.

分会场报告 5

S10-1 有限体积法理论及其应用

Linear and Quadratic Immersed Finite Element Methods for the Multilayer Porous Wall Model

林延平²⁰⁴

Abstract: We consider a simple multi-layer porous wall model for coronary drug-eluting stents which contains not only several discontinuous coefficients interface points, but also the imperfect contact interface point. We construct the general linear and quadratic immersed finite element methods for solving it. The optimal error estimates in L_2 and H_1 norm for both IFE methods are derived. Finally some numerical tests are provided to confirm theoretical prediction.

²⁰² 李猛, 华中科技大学. Email: limeng_zzu@163.com

²⁰³ 纪翠翠, 东南大学. Email: cuicuihuan@163.com

²⁰⁴ 林延平, 香港理工大学.

On the locally conserving flux derived from a finite element solution

邹青松²⁰⁵

Abstract: In this talk, we will present two approaches to derive locally conserving flux from a continuous Galerkin finite element solution (CG-FEM). By one approach, we obtain elementwisely conserving flux while by the other approach, we obtain volumewisely conserving flux. Both two post-processing approach require only to solve a smaller linear system on each element of the underlying mesh. Moreover, both our theoretical reasoning and numerical experiments show that the derived numerical flux converges to the exact flux with optimal order.

L^2 error estimate and superconvergence of high order finite volume methods on triangular meshes

Xiang Wang, Yonghai Li²⁰⁶

Abstract: We established a unified framework of the L^2 error estimate for arbitrary order FVM on triangular meshes. Orthogonal conditions are originally proposed to construct the dual meshes, which guarantee the optimal convergence rate with L^2 norm of the corresponding FVM schemes. Moreover, with the orthogonal conditions, we established the superconvergence theory for quadratic FVM on triangular meshes.

A family of vertex-centered linearity-preserving schemes for diffusion problems on arbitrary polygonal meshes

邬吉明²⁰⁷

Abstract: We suggest a family of vertex-centered linearity-preserving finite volume schemes for the heterogeneous anisotropic diffusion equations on general polygonal meshes. The unknowns of these schemes are defined at the mesh vertices, and no auxiliary unknowns are utilized. The schemes are locally conservative with respect to the dual mesh, capture exactly the linear solutions, lead to symmetric positive definite linear systems, and yield a nine-point stencil on structured quadrilateral meshes. The coercivity, stability and H^1 error estimate of the schemes are rigorously analyzed on arbitrary mesh size under some weak geometry assumptions. Also the relation with the finite volume element method is discussed. Finally some numerical tests show the optimal convergence rates for the discrete solution and flux on various mesh types and for various diffusion tensors.

²⁰⁵ 邹青松, 中山大学. Email: mcszqs@mail.sysu.edu.cn

²⁰⁶ 王翔, 吉林大学. Email: wxjdx@jlu.edu.cn

²⁰⁷ 邬吉明, 北京应用物理与计算数学研究所.

Energy-Preserving Finite Volume Element Method for the Boussinesq equations

张志跃²⁰⁸

Abstract: In this talk, some finite volume element schemes are proposed for solving the "good" and improved Boussinesq equations. The energy-preserving scheme are designed by using the discrete variational derivative method to inherit the conservation properties from the equation. The energy-preserving scheme can conserve the discrete mass and energy to the machine precision. The standard finite volume element scheme can conserve the discrete mass to the machine precision. The proposed schemes all have good convergence performances when choose large mesh size for a long time computation. Numerical experiments illustrate the effectiveness of proposed schemes.

S12-1 稀有事件及其鞍点问题的计算与应用

Theoretical and Numerical Advancement for Transition State Calculations in Rare-event Study

周翔²⁰⁹

Abstract: The transition states on potential energy surface belong to a class of special saddle points having only one unstable direction. They play key roles in the understanding the rare events like phase transitions and noise-induced transitions escaping a stable point. Many existing methods like dimer method have been widely used for finding transition state by local search. Here we review our work on theoretic and numerical progresses: the gentlest ascent dynamics (Nonlinearity, vol. 24, pp. 1831, 2011) and the iterative minimization algorithm (J. Comp. Phys. vol 309, pp 69-87. 2016). We also introduce the improvement for spatially-extended models by the aid of convex splitting method (with Shuting Gu0. The work is supported by HK GRF 11304715.

²⁰⁸ 张志跃, 南京师范大学. Email: zhangzhiyue@njnu.edu.cn

²⁰⁹ 周翔, 香港城市大学. Email: zhou.xiangni@gmail.com

芽殖酵母细胞周期 S 期检验点激活的稀有事件研究

李铁军²¹⁰

Abstract: 对于芽殖酵母细胞周期中 DNA 损伤的研究是系统生物学中的一个重要课题, 并已经得到实验生物学家的相当探讨。以往研究基本关注于定性的讨论和对于 DNA 损伤通路的探索, 定量的研究较少。通过与生物物理学家合作, 对得到的实验数据进行分析, 我们较为定量的研究了由于药物刺激而导致的芽殖酵母细胞周期 S 期检验点激活的过程并进行了相应的模型研究。我们的研究表明, 稀有事件是理解这一激活过程内在机理的理论基础。

The equilibrium melting path of the hexagonal ice

汪涵²¹¹

Abstract: Water is one of the most common materials on earth, but the understanding of the microscopic mechanism of the ice melting is still lacking. The ice melting is a typical rare event: the time spend by the system in the ice state is orders of magnitude longer than the transition time to the liquid state, which leads to a substantial difficulty for the microscopic simulation techniques like the molecular dynamics simulation. In this talk, the computation of the equilibrium melting path is made possible by coupling the string method with the molecular dynamics. We investigate the microscopic mechanism of the formation of the liquid nucleus in the bulk hexagonal ice, and disclose a different scenario from the classical nucleation theory at the early stage of the melting. The new techniques that accelerate the molecular dynamics simulation are also introduced in this talk.

Convergence Analysis of a Minimum Action Method for Non-gradient Systems

于海军²¹²

Abstract: In this talk, we address the convergence of the finite element approximation of the minimizer of Freidlin-Wentzell (F-W) action functional. The F-W theory of large deviations is a rigorous mathematical tool to study small-noise-induced transitions in a dynamical system. The central task in the application of F-W theory of large deviations is to seek the minimizer and minimum of the F-W action functional. We discretize the F-W action functional using linear finite element, and establish the convergence of the approximated minimizer through Γ -convergence. This talk based on a joint work with Xiaolaing Wan(LSU) and Jiayu Zhai(LSU).

²¹⁰李铁军, 北京大学. Email: tieli@pku.edu.cn

²¹¹汪涵, 北京应用物理与计算数学研究所.

²¹²于海军, 中科院计算数学所. Email: hyu@lsec.cc.ac.cn

Glassy dynamics, spinodal fluctuations, and the kinetic limit of nucleation in suspensions of colloidal hard rods

Ran NI²¹³

Abstract: Using simulations we identify three dynamic regimes in supersaturated isotropic fluid states of short hard rods: (i) for moderate supersaturations, we observe nucleation of multi-layered crystalline clusters; (ii) at higher supersaturation, we find nucleation of small crystallites which arrange into long-lived locally favored structures that get kinetically arrested; and (iii) at even higher supersaturation, the dynamic arrest is due to the conventional cage-trapping glass transition. For longer rods we find that the formation of the (stable) smectic phase out of a supersaturated isotropic state is strongly suppressed by an isotropic-nematic spinodal instability that causes huge spinodal-like orientation fluctuations with nematic clusters diverging in size. Our results show that glassy dynamics and spinodal instabilities set kinetic limits to nucleation in highly supersaturated hard-rod fluids.

T02-1 流体力学中的数值计算

Second order time-space iterative method for the stationary Navier-Stokes equations

黄鹏展, 何银年, 冯新龙²¹⁴

Abstract: A second order time-space implicit/explicit iterative scheme for the stationary Navier-Stokes equations is designed, where the spatial discretization is based on the mixed finite element method and the time discretization is based on the second order implicit/explicit (the Crank-Nicolson/Admas-Bashforth) scheme. Under a weak uniqueness condition, the optimal H^1 - L^2 error estimates related to the mesh size h and time step size τ of the iterative solution (u_h^n, p_h^n) to the exact solution (u, \tilde{p}) and the optimal L^2 error estimate related to h and τ of the iterative solution u_h^n to the exact solution u are provided. In numerical aspect, some comparisons with the first order time-space iterative method are made to confirm the efficiency of the proposed second order scheme.

²¹³Ran NI, Nanyang Technological University.

²¹⁴黄鹏展, 新疆大学数学与系统科学学院. Email: hpzh007@yahoo.com

溃坝流问题的改进 SPH 方法模拟

许晓阳²¹⁵

Abstract: 作为一种典型的自由表面流问题，溃坝流的数值模拟一直备受广大科研人员的关注和重视。但由于此类问题的自由面往往伴随有飞溅、翻转、破碎等不连续流动特征，因此对传统的网格类方法来说极具挑战性。本报告介绍了一种改进的光滑粒子动力学 (Smoothed particle hydrodynamics, SPH) 方法用于模拟三维复杂溃坝流问题。改进的 SPH 方法包括：施加核梯度修正技术以提高 SPH 方法的计算精度；在连续性方程中通过加入 Rusanov 通量以消除 SPH 方法的压力不稳定性问题。应用改进 SPH 方法对多种复杂溃坝流问题进行了三维数值模拟，数值结果与实验数据吻合较好。计算结果表明，该改进 SPH 方法能逼真地复现了坝内水体与壁面间相互作用而产生的多种复杂物理现象，且能得到传统 SPH 方法所不能模拟得到的数值结果。

不同三维网格下的拉氏流体数值分析

徐骁，高志明，戴自换²¹⁶

Abstract: 为了提高网格适应性以及计算效率，通常在计算中采用多块网格或非结构网格。然而，多块网格界面附近的尺度非均匀性及非结构网格中四面体排列方式会对格式的计算精度产生较大地影响。本文基于三维拉氏单元中心格式，通过经典算例分别研究不同类型网格对计算精度、效率等方面的影响。结果表明，相较于六面体网格和射线型网格，分块网格可以保证较高的计算精度以及效率，但在流场中出现强间断时，由于分块界面两端网格尺度非均匀性会产生较大的误差。非结构网格中四面体的排列方式会影响网格的方向性，当采用六面体剖分为 24 个四面体的网格时，由于具有良好的结构对称性，其计算结果精度远高于将六面体剖分为 5 个或 6 个四面体的网格。

²¹⁵许晓阳, 陕西理工大学. Email: xiaoyang.xu@snut.edu.cn

²¹⁶徐骁, 北京应用物理与计算数学研究所. Email: xu_xiao@iapcm.ac.cn

Linear, Second Order and Unconditionally Energy Stable Schemes for a hydrodynamic model of Smectic-A Liquid Crystals

Rui Chen²¹⁷

Abstract: Here we consider the numerical approximations for a hydrodynamical model of smectic-A liquid crystals. The model, derived from the variational approach of the modified Oseen-Frank energy, is a highly nonlinear system that couples the incompressible Navier-Stokes equations and a constitutive equation for the layer variable. We develop two linear, second-order time-marching schemes based on the “Invariant Energy Quadratization” method for nonlinear terms in the constitutive equation, the projection method for the Navier-Stokes equations, and some subtle implicit-explicit treatments for the convective and stress terms. Moreover, we prove the well-posedness of the linear system and their unconditionally energy stabilities rigorously. Various numerical experiments are presented to demonstrate the stability and the accuracy of the numerical schemes in simulating the dynamics under shear flow and the magnetic field.

An efficient exponential integrator factor method with non-polynomial direct discontinuous Galerkin spatial approximation for solving viscous Burgers’ equations

Yaru Cao, Liyong Zhu²¹⁸

Abstract: In this talk, we present an efficient exponential integrator factor method for solving Burgers’ equations with small viscous coefficient. It is well known that the boundary layer will be produced when the viscous coefficient is sufficiently small, and this makes the solution to this equation difficult. Rather than employing the traditional Runge-Kutta direct discontinuous Galerkin (RKDDG) method based on piecewise polynomial space, the proposed method using the DDG method based on the exponential basis to perform the spatial direction discretization in the boundary layer while the Runge-Kutta exponential integrator factor method is employed to perform the temporal direction discretization. Numerical examples illustrate that, compared to the traditional DDG method, the developed method not only provide the better spatial approximation even if on a rather coarse spatial grid in the boundary layer, but also permit larger time step.

Enriched Finite Element Methods for Stokes Interface Problems

Hua Wang, Jinru Chen²¹⁹

Abstract: We propose a conforming enriched finite element method for Stokes interface problems with interface-unfitted meshes. Optimal convergence rates are obtained.

²¹⁷ 陈锐, 北京应用物理与计算数学研究所. Email: micerui@tom.com

²¹⁸ 曹雅茹, 北京航空航天大学. Email: 1264487629@qq.com

²¹⁹ 王华, 南京师范大学. Email: sky_wanghua@163.com

粘弹性流动问题非结构网格有限体积法的高效求解

赵立飞, 欧阳洁, 周文, 解岩, 苏进²²⁰

Abstract: 基于粘弹性流动问题, 在非结构网格上, 本文发展了一种高效的代数求解器, 即耦合非结构网格有限体积方法的简化最小残量方法 (SGMRES(m))。其中, SGMRES(m) 方法用于求解大型稀疏变系数线性方程组, 该方程组由非结构网格有限体积方法离散粘弹性控制方程导出。针对基于 Oldroyd-B 本构的粘弹性流体, 应用 SGMRES(m) 耦合非结构有限体积方法, 模拟得到的管道流应力的数值结果与解析解吻合很好, 并且圆柱绕流曳力系数的模拟结果与文献值吻合得也很好, 验证了该求解器的有效性。本文还在这两个算例中比较了同样精度下, 不同求解器下的 CPU 时间, 结果表明该求解器的耗时最短, 从而验证了该求解器的高效性。

T04-1 数值代数

A Riemannian Newton Method for Nonnegative Inverse Eigenvalue Problems

Zhi Zhao, Zheng-Jian Bai, and Xiao-Qing Jin²²¹

Abstract: In this talk, we consider the nonnegative inverse eigenvalue problem of finding a nonnegative matrix such that its spectrum is the prescribed self-conjugate set of complex numbers. We reformulate the nonnegative inverse eigenvalue problem as an underdetermined constrained nonlinear matrix equation over several matrix manifolds. Then we propose a Riemannian Newton-type method for solving the nonlinear matrix equation. The global and quadratic convergence of the proposed method is established. Finally, we report some numerical experiments to illustrate the efficiency of the proposed method.

Jacobi-Like Algorithm for Bethe-Salpeter Eigenvalue Problem

Weiguo Gao²²²

Abstract: In this talk, we investigate the Bethe-Salpeter eigenvalue problems and propose a Jacobi-like algorithm. The eigen-structure is preserved during the iterations. Global convergence of the new algorithm is given and numerical examples demonstrate the fast convergence. This is joint work with Meiyue Shao and Cheming Yang.

²²⁰ 赵立飞, 西北工业大学. Email: zhaolf100@163.com

²²¹ 白正简, 厦门大学. Email: zjbai@xmu.edu.cn

²²² 高卫国, 复旦大学. Email: wggao@fudan.edu.cn

Multi-step modified Newton-NSS method for solving systems of nonlinear equations

Qingbiao Wu, Pingfei Dai²²³

Abstract: The Normal and skew-Hermitian splitting (NSS) method converges unconditionally to the exact solution of the system of linear equations, we establish a class of multi-step modified Newton-NSS method for solving large sparse systems of nonlinear equations with positive definite Jacobian matrices at the solution points. Under proper conditions, the local convergence theorem is proved. Further, the successiveoverrelaxation (SOR) technique has been proved quite successfully in accelerating the convergence rate of the NSS or the Hermitian and skew-Hermitian splitting (HSS) iteration method, so we employ the SOR method in the NSS iteration, then we get a new method, called as multi-step modified Newton SNSS, and numerical results are given to confirm the effectiveness of our methods.

The convergence theory for the restricted version of the overlapping Schur complement preconditioner

Xin Lu, Xing-ping Liu and Tong-xiang Gu²²⁴

Abstract: The restricted version of the overlapping Schur complement (SchurRAS) preconditioner was introduced by Li and Saad [SIAM J. Sci. Comput., 27(2006), pp. 1787–1801] for the solution of linear system $Ax = b$, and numerical results have shown that the SchurRAS method outperforms the restricted additive Schwarz (RAS) method both in terms of iteration count and CPU time. In this paper, based on meticulous derivation, we give an algebraic representation of the SchurRAS preconditioner, and prove that the SchurRAS method is convergent under the condition that A is an M -matrix and it converges faster than the RAS (restricted additive Schwarz) method.

Markovian 二叉树中二次向量方程的算法

郭培昌, 徐树方²²⁵

Abstract: 我们将介绍 Markovian 二叉树中二次向量方程已有的算法, 并报告我们最新的研究进展。我们将介绍 Newton-Shamanskii 类型算法, 证明了, Newton-Shamanskii 算法产生的向量序列是单调递增的, 具有大范围收敛性。数值实验展示了算法的有效性。

²²³ 吴庆标, 浙江大学数学科学学院. Email: qbwu@zju.edu.cn

²²⁴ 卢欣, 中国石油大学(北京). Email: inbelief@163.com

²²⁵ 郭培昌, 中国地质大学(北京). Email: gpeichang@126.com

GMRES Method for Multi-Scattering Problems

RuiZhang (Hunan Normal University)²²⁶

Abstract: In this talk, we introduce a GMRES iterative method to solve the multi-scattering problems. Instead of solving the density in integral equation in traditional Boundary Element method, we hope to obtain the purely out-going waves of each scatter by solving a series of local scattering problems (local solvers) with single scatter in each iteration of GMRES. Then we can derive the global scattering field by addition theorem. We choose the Spectral Element method with DtN condition as the local solvers, and we find that the iterate steps are independent on the degree of freedom of each local solver. We also give the convergence analysis, and some numerical examples to illustrate our results.

(Joint work with BoWang and ZiqingXie)

On a simpler SSOR-like method for augmented systems

Huidi, Wang, Zhengda, Huang²²⁷

Abstract: In this talk, we propose a new SSOR-like method with four parameters to solve the augmented system. And we analyze the convergence of the method and get the optimal convergence factor under suitable conditions. It is proved that the optimal convergence factor is the same as the GMPD method [M.A. Louka and N.M. Missirlis, A comparison of the extrapolated successive overrelaxation and the preconditioned simultaneous displacement methods for augmented systems, Numer. Math. 131(2015) 517-540] with five parameters under the same assumption, and that the optimal convergent parameters of the SSOR-like methods are not unique. So we discuss the selection of the optimal parameters of the SSOR-like methods in the numerical experiments.

²²⁶ 张瑞, 湖南师范大学. Email: 1454176705@qq.com

²²⁷ 王会迪, 浙江大学数学科学学院. Email: hdwang@zju.edu.cn

T06-5 有限元和边界元方法

Virtual Element Methods for Obstacle Problem

Fei Wang (王飞)²²⁸

Abstract: We study virtual element methods for solving obstacle problem, which is a representative elliptic variational inequality of the first kind. The virtual element methods (VEMs) can be regarded as a generalization of the standard finite element methods with addition of some suitable non-polynomial functions, and the degrees of freedom are carefully chosen so that the stiffness matrix can be computed without actually computing the non-polynomial functions. With this special design, the virtual element methods can easily deal with complicated element geometries. In this paper, we establish a priori error estimates of the virtual element methods for the obstacle problem. We prove that the lowest order VEMs achieve the optimal convergence rate. Some numerical examples are reported to show that the virtual element methods can work on very general polygonal elements, and the convergence rate in H^1 norm matches well with the theoretical prediction.

多孔弹性模型多物理场有限元方法

葛志昊²²⁹

Abstract: 多孔弹性模型是孔隙尺度下流体-固体相互作用的系统,是连续介质力学和声学的一个非常重要的分支,在油藏工程、材料、土壤力学、生物医药、环境工程、地震工程等工程技术领域有广泛应用。由于多孔弹性模型本身非常复杂,加上求解区域几何形状不规则,所以求其解析解极其困难,因此,求解此类问题只能依赖数值计算,通常采用有限元方法,然而现有文献均直接逼近原始模型会产生“闭锁现象”。于是,发展高效稳定的数值方法显得越来越重要了。我们初步的研究结果发现对于准静态的线性多孔弹性模型可以引入变量对模型重建,不仅清楚地揭示了多物理过程而且设计的多物理场有限元方法成功克服了“闭锁现象”。

²²⁸ 王飞, 西安交通大学. Email: feiwang.xjtu@xjtu.edu.cn²²⁹ 葛志昊, 河南大学. Email: zhihaoge@henu.edu.cn

Navier-Stokes 方程：局部间断 Galerkin 方法，非线性稳定性，收敛性。

王淑琴²³⁰

Abstract: By combining the characteristic method and the local discontinuous Galerkin method with carefully constructing numerical fluxes, variational formulations are established for time-dependent incompressible Navier-Stokes equations in \mathbb{R}^2 . The nonlinear stability is proved for the proposed symmetric variational formulation. Moreover, for general triangulations the priori estimates for the L^2 -norm of the errors in both velocity and pressure are derived. Some numerical experiments are performed to verify theoretical results.

Local discontinuous Galerkin methods with implicit-explicit time-marching for time-dependent incompressible fluid flow

Haijin Wang, Yunxian Liu, Qiang Zhang, Chi-Wang Shu²³¹

Abstract: In this talk we will give the stability and error estimates of the local discontinuous Galerkin (LDG) methods coupled with multi-step implicit-explicit (IMEX) time discretization schemes, for solving time-dependent incompressible fluid flows. We will give theoretical analysis for the Oseen equation, and assess the performance of the schemes for incompressible Navier-Stokes equations numerically. For the Oseen equation, we show the first order IMEX-LDG scheme is unconditionally stable for Q_k elements on cartesian meshes, and by the aid of the Stokes projection and inf-sup condition, we obtain the optimal error estimates for the velocity, the stress (gradient of velocity) and the pressure, in both space and time.

T08-1 自适应方法

An h-adaptive RKDG method and its applications

朱洪强²³²

Abstract: In this talk we present an h-adaptive Runge-Kutta discontinuous Galerkin method which is based on mesh refinement and coarsening. First, the framework of this method is presented, together with the implementation details. After that, we show its applications to different problems, including hyperbolic conservation laws, detonation wave simulations and Vlasov-Poisson system. Numerical results of classical test problems are given to illustrate the effectiveness and the capability of this method.

²³⁰ 王淑琴, 西北工业大学. Email: wangshuqin@nwpu.edu.cn

²³¹ 王海金, 南京邮电大学. Email: hjwang@njupt.edu.cn

²³² 朱洪强, 南京邮电大学. Email: zhuhq@njupt.edu.cn

A Convergent Adaptive Finite Element Method for Elliptic Dirichlet Boundary Control Problems

龚伟²³³

Abstract: In this talk we consider the adaptive finite element method for elliptic Dirichlet boundary control problems in energy space. Firstly, we rigorously derive efficient and reliable a posteriori error estimates for finite element approximations of the Dirichlet boundary control problems. As a byproduct, a priori error estimates can be derived in a simple way by introducing appropriate auxiliary problems and establishing certain norm equivalence. Secondly, for the coupled elliptic partial differential system involving the control, the state and the adjoint state which resulted from the first order optimality system, we prove that the sequence of adaptively generated discrete solutions, guided by our newly derived a posteriori error indicators, converge to the true solutions along with the convergence of the error estimators.

Adaptive finite element methods for scattering problems in unbounded domain

Junliang Lv²³⁴

Abstract: In this talk, I will give some recent work on scattering problems. One of main difficulties for solving these problems with finite element methods is the unboundedness of physical domains. Two effective strategies to truncate these unbounded domains into bounded computable domains are introduced. One is the transparent boundary condition (TBC) approach, the other is the perfectly matched layer (PML) technique. Moreover, Adaptive mesh refinement methods based on the a posteriori estimates are considered to deal with complex problem geometries and potential discontinuous material parameters. Some numerical results will be presented to illustrate the competitive behavior of the proposed method.

²³³ 龚伟, 中科院数学与系统科学研究院. Email: wgong@lsec.cc.ac.cn

²³⁴ 吕俊良, 吉林大学. Email: lvjl@jlu.edu.cn

A parameter-uniform adaptive grid method for singularly perturbed parabolic convection-diffusion problems

Li-Bin Liu, Yanping Chen²³⁵

Abstract: A parameter-uniform adaptive grid method is proposed to solve a singularly perturbed parabolic convection-diffusion problem. Firstly, the domain is discretized with a uniform mesh on the time direction and a nonuniform grid obtained by equidistributing a positive monitor function on the spatial variable. It is shown that the discrete numerical solution obtained by the implicit Euler scheme for the time derivative and the upwind finite difference scheme for the spatial derivative. Then, an a posteriori error estimate is derived for the presented adaptive grid method. In addition, the uniform convergence based on discrete Green function for the fully discrete scheme is also proved. Furthermore, some nonlinear singular perturbation parabolic convection-diffusion problem also studied. At last, some numerical results are given to validate the theoretical results.

An h - p Version Of The Continuous Petrov-Galerkin Method For Volterra Delay-Integro-Differential Equations

王利娜, 易利军²³⁶

Abstract: We consider an h - p version of the continuous Petrov-Galerkin time stepping method for Volterra integro-differential equations with proportional delays. We derive a priori error bounds in the L^2 -, H^1 - and L^∞ -norm that are explicit in the local time steps, the local approximation orders, and the local regularity of the exact solution. Numerical experiments are presented to illustrate the theoretical results.

²³⁵ 刘利斌, 广西师范学院. Email: liulibin969@163.com

²³⁶ 王利娜, 上海师范大学. Email: 1842988390@qq.com

T10-1 随机微分方程**Hybrid Monte Carlo Acceleration Method for Pricing European Options under Levy Processes**徐承龙, 孙永超²³⁷

Abstract: This paper constructs an efficient hybrid Monte Carlo variance reduction method for pricing European options driven by Levy process. The hybrid variance reduction method combines conditional Monte Carlo(CMC) and importance sampling(IS) technique. Owing to the structure of movement of asset price and Black-Scholes formula, we formulate the conditional expectation of the European option price under Levy process and then the IS method is used to reduce simulation variance greatly. Since the conditional expectation formula is smooth with respect to(w.r.t) the concerned parameters, the Greeks, which means the gradient of the option price to the parameters, can be calculated conveniently and efficiently. Furthermore, we proposed a very efficient prediction-correction algorithm to determine the optimal parameters in the importance sampling measure based on the moments match idea and iteration correction algorithm. Numerical examples confirm that our hybrid acceleration method has reasonable variance reduction effect and the prediction-correction algorithm determining the optimal parameters in the importance sampling measure can save a lot of time cost than the traditional Newton's iteration method. Some theoretical results are also given such as convergence of sample average approximation (SAA) method and the existence and uniqueness of the optimal problem determining the parameters in the importance sampling measure.

²³⁷ 徐承龙, 同济大学. Email: clxu@tongji.edu.cn

Variable-separation methods based on sparse and low rank representation for stochastic partial differential equations

姜立建, 李秋齐²³⁸

Abstract: In this talk, we present a novel variable-separation (VS) method for generic multivariate functions. The idea of the novel VS is extended to obtain the solution in tensor product structure for stochastic partial differential equations (SPDEs). Compared with many widely used variation-separation methods, the novel VS shares their merits but has less computation complexity and better efficiency. The novel VS can be used to get the separated representation of the solution for SPDE in a systematic enrichment manner. No iteration is performed at each enrichment step. This is a significant improvement compared with proper generalized decomposition. Because the stochastic functions of the separated representations obtained by the novel VS depend on the previous terms, this impacts on the computation efficiency and brings great challenge for numerical simulation for the problems in high stochastic dimensional spaces. In order to overcome the difficulty, we propose an improved least angle regression algorithm (ILARS) and a hierarchical sparse low rank tensor approximation (HSLRTA) method based on sparse regularization. For ILARS, we explicitly give the selection of the optimal regularization parameters at each step based on least angle regression algorithm (LARS) for lasso problems such that ILARS is much more efficient. HSLRTA hierarchically decomposes a high dimensional problem into low-dimensional problems and brings an accurate approximation for the solution to SPDEs in high dimensional stochastic spaces using limited computer resource. Some examples are presented to illustrate the efficacy of the proposed methods.

超线性随机微分方程的数值方法

郭谦、刘晔、毛学荣等²³⁹

Abstract: 在运用经典显格式求解超线性随机微分方程时, 数值解无法收敛到原方程的解。我们主要构造一类截断方法, 该类方法得到的数值解可以有效逼近原问题的解, 不仅在有限时间内保证解的收敛性, 还能在一定条件下再现真解的稳定性和有界性。该方法进一步被推广到弱收敛的情形, 结合多水平 Monte-Carlo 方法提高计算效率。

²³⁸姜立建, 湖南大学. Email: ljjiang@hnu.edu.cn

²³⁹郭谦, 上海师范大学. Email: qguo@shnu.edu.cn

Mean square stability of semi-implicit Euler method for nonlinear neutral stochastic delay integro differential equations

Yuan Haiyan²⁴⁰

Abstract: This paper deals with the mean-square stability of semi-implicit Euler method for nonlinear neutral stochastic delay integro-differential equations. It is shown that the semi-implicit Euler method inherits the mean-square stability property of the analytic system. Moreover, the semi-implicit Euler method is mean square stable with no restrictions on the step size. In addition, numerical experiments are presented to confirm the theoretical results.

Generator approximation method for solving forward backward stochastic differential equations and its applications

付余, 赵卫东, 周涛²⁴¹

Abstract: Generator approximation method was firstly proposed for numerically solving coupled forward backward stochastic differential equations in 2014. Our recent studies have extended its applications to solve FBSDEs with jumps and stochastic optimal control problems. In this talk, we introduce the general method of the generator approximations for FBSDEs with jumps and propose the multistep schemes. The most important advantage of the multistep scheme is that highly accurate numerical solutions can be obtained for the BSDE, which are usually our quantities of interest, while the forward SDE is solved by the simplest Euler scheme with only one jump therein. This feature leads to a dimension reduction when calculating the stochastic integral with respect to Poisson random measure, which greatly reduces the computational complexity and shows a very promising prospect for solving high-dimensional FBSDEs.

Stability of a class of hybrid stochastic neutral differential equations with unbounded delay

Lu Boliang, Song Ruili (逯伯亮, 宋瑞丽)²⁴²

Abstract: 报告主要介绍带 Markov 切换的中立型无界时滞随机微分方程解的稳定性研究。近年来混合型随机动力系统在机械工程、化学工程、生物技术、金融领以及管理科学等领域有着非常广泛的应用, 随机微分方程作为概率论与微分方程理论的结合, 受到了广大学者的关注。作者在已有的结果基础上, 将时滞项从常数时滞和有界时滞推广到无界时滞的情形, 得出了解的 p -阶矩指数稳定和几乎处处指数稳定结论。希望在本次报告中, 可以就此与各位老师同学学习交流。

²⁴⁰ 袁海燕, 黑龙江工程学院. Email: yhy82_47@163.com

²⁴¹ 付余, 山东科技大学. Email: nielf_fu@sdust.edu.cn

²⁴² 逯伯亮, 南京财经大学. Email: luboliangybfq@126.com

Stochastic Collocation via nonconvex compressive sensing and its application to solve SPDEs with random inputs

Ling Guo, Yongle Liu, Liang Yan²⁴³

Abstract: In this paper, we consider the stochastic collocation method via non-convex compressive sensing methods, mainly including L_q minimization and transformed L_1 (for short, TL1) minimization, and their applications in partial differential equations with random inputs. The main results of this paper can be listed as the following two parts: 1) By using the norm inequality between L_q and L_2 and the square root lifting inequality, we present several new theoretical estimates regarding the recoverability for both sparse and non-sparse signals via L_q minimization. At the same time, based on the work of Candes, we establish new results of TL1 minimization about the accuracy of the reconstruction from underdetermined measurements which improve on the earlier estimates derived by Zhang and Xin, and have the advantage of being more elegant. 2) We then combine this method with the stochastic collocation to identify the coefficients of sparse orthogonal polynomial expansions, stemming from the field of uncertainty quantification. We obtain recoverability results for both sparse polynomial functions and general non-sparse functions. We also present various numerical experiments to show the performance of the L_q and TL1 algorithm. In each part, we first present some bench mark tests to demonstrate the ability of L_q and TL1 minimization to recover exactly sparse signals, and then consider using the orthonormal polynomials expansions to approximate some classical analytical functions, and present the advantage of this method over other optimization methods (for example, standard L_1 , reweighted L_1 minimization, L_1 – L_2 minimization). Finally, both partial differential equations and ordinary differential equations with random inputs are considered and we compare the approximation error of our quantity of interest (QoI) in the numerical experiments. All the numerical results indicate that the L_q method performs better than standard L_1 and reweighted L_1 minimization. As for the TL1 method, it also outperforms than standard L_1 and L_1 – L_2 minimization.

²⁴³刘永乐, 上海师范大学. Email: yololiu@163.com

T11-1 有限差分法及其应用

三维扩散方程的金字塔格式

杭旭登, 王帅, 袁光伟²⁴⁴

Abstract: 我们提出了三维扩散方程在一般多面体单元上的一种新型的单元中心格式, 称为金字塔格式 (P 格式). 格式针对一般的具有非平的表面的多面体单元设计. 表面上的单位外法向流在一个优化选择的等效平面上离散. 单位外法向流的离散表达式只是涉及单元中心和单元角点, 而无需单元表面的中心量. 特别, 对于表面非平的六面体单元, 离散流的表达式非常简单. 和已有的二阶精度格式相比, 新的格式的离散计算量非常低, 并且更健壮. 数值结果表明算法有很好的计算精度.

求解带有不连续系数和非奇异源项的 Helmholtz 方程的高阶紧致格式

曹娇娇, 冯秀芳²⁴⁵

Abstract: 在实际应用中对于各种波的数值求解, 由于波数的不同都可归结为由带有不连续系数的椭圆型方程来描述. 一些研究者分别利用有限差分、有限体积和有限元等计算方法对这类问题做了大量工作. 由界面问题所导出的偏微分方程的解在通过间断界面时一般是不连续的, 这使得大多数常规的求解偏微分方程的数值解法不能很好的适用于求解界面问题, 而有限体积方法因其保持物理量的局部守恒性、计算简单而成为解决界面问题的有效方法. 本文主要是结合有限体积法和有限差分法对二维带有不连续系数和非奇异源项的 Helmholtz 方程进行离散, 得到一类高阶紧致差分格式, 通过数值算例验证了方法的有效性.

²⁴⁴ 杭旭登, 北京应用物理与计算数学研究所. Email: hang_xudeng@iapcm.ac.cn

²⁴⁵ 冯秀芳, 宁夏大学. Email: xf_feng@nxu.edu.cn

Energy conservation and super convergence analysis of the EC-S-FDTD method for Maxwell equations with periodic boundaries

Liping Gao, Rengang Shi and Hui Guo²⁴⁶

Abstract: This talk is concerned with new energy analysis of the two dimensional (2D) Maxwell equations and the symmetric energy-conserved splitting finite difference time domain (EC-S-FDTD) method with the periodic boundary condition(PBC). New energy identities of the Maxwell equations in H^2 norm are proposed and interpreted by considering the physical meanings of the H^1 and H^2 semi-norms. It is shown that the curls of the electromagnetic fields are conserved in terms their magnitudes. By the new energy methods, the numerical energy identities of the symmetric EC-S-FDTD method are derived and shown that the symmetric EC-S-FDTD scheme is unconditionally stable and convergent to the continuous identities. By error estimate it is proved that the symmetric EC-S-FDTD method with PBC is of second order (super) convergence in the discrete H^1 and H^2 norms. Numerical experiments are carried out and confirm the analysis on energy conservation, stability and super convergence.

Conservative modified Crank–Nicolson and time-splitting wavelet methods for modeling Bose–Einstein condensates in delta potentials

钱旭²⁴⁷

Abstract: This talk explores two wavelet-based energy-conserving algorithms for the Gross–Pitaevskii equation with delta potentials in Bose–Einstein condensates, named modified Crank–Nicolson wavelet method and time-splitting wavelet method, respectively. Both proposed methods can preserve the intrinsic properties of original problems as much as possible. Meanwhile, the rigorous error estimates and some conservative properties are investigated. They are proved to preserve the charge conservation exactly. The global energy conservation laws can be preserved under several conditions. In practical computations, to avoid a large drift in energy values caused by discontinuous potential well, an improved discrete delta function is implemented. Numerical experiments for attractive and repulsive cases are conducted during long time computations to show the performances of the proposed methods and verify the theoretical analysis.

²⁴⁶高理平, 中国石油大学(华东)理学院. Email: l.gao@upc.edu.cn

²⁴⁷钱旭, 国防科学技术大学. Email: qianxu@nudt.edu.cn

Some numerical researches on split-step methods

王姗姗²⁴⁸

Abstract: The split-step method is efficient for multi-dimensional problems of parabolic or Schrodinger-type equations. In this talk, several split-step methods are introduced, which involve split-step orthogonal spline collocation methods for multi-dimensional nonlinear Schrodinger (NLS) equations, split-step compact finite difference methods for cubic-quintic complex Ginzburg-Landau equations, split-step cubic B-spline collocation methods for NLS equation. Interesting numerical tests are carried out to show that these methods are efficient and superior.

conservative compact difference scheme for the zakharov equaiton

周旋旋, 张鲁明²⁴⁹

Abstract: In this paper, we present a conservative fourth-order compact difference scheme for the initial-boundary value problem of the Zakharov equations. Discrete conservation laws, convergence and stability of the new scheme are proved by energy method. Several numerical results are reported to support our theoretical analysis.

求解三维变系数 Helmholtz 方程的高阶紧致差分格式

鲜双燕²⁵⁰

Abstract: 本文构造了求解三维变系数 Helmholtz 方程的四阶紧致差分格式. 首先利用中心差分方法离散原方程得到二阶紧致差分格式, 然后利用 Taylor 展开式对二阶格式的截断误差项进行修正, 得到求解三维变系数 Helmholtz 方程的四阶紧致差分格式. 最后采用循环的广义极小残余算 (GMRES(m)) 算法对方程组进行求解, 数值结果验证了文中构造格式的有效性和可行性, 通过对直接方法和 GMRES(m) 方法的计算时间做的比较, 表明对三维变系数 Helmholtz 方程的求解, GMRES(m) 算法的优势明显

²⁴⁸ 王姗姗, 南京航空航天大学. Email: wangss@nuaa.edu.cn

²⁴⁹ 周旋旋, 南京航空航天大学. Email: 867928563@qq.com

²⁵⁰ 鲜双燕, 宁夏大学. Email: 1306787183@qq.com

T12-1 移动网格和无网格及有限体积法

Analysis of two moving least squares approximation-based meshless methods

李小林²⁵¹

Abstract: Meshless (or meshfree) methods, that only require a cluster of scattered nodes rather than elements to be specified in the physical domain, have tremendous potential advantages over traditional mesh-based numerical methods such as the finite element method that require discretization of a body into elements. The basis of meshless methods is shape functions. The moving least squares (MLS) approximation is an important method to form shape functions in meshless methods. For the application of MLS-based meshless methods to the numerical solution of boundary value problems, it is fundamental to analyze the MLS approximation. This report begins by discussing error estimates of the MLS approximation. The element-free Galerkin (EFG) method is a typical domain-type meshless method based on coupling the MLS approximation and the global Galerkin weak form. Error analysis of the EFG method is then provided theoretically. To retain the merits of both the boundary element method in dimension reduction and the meshless method in elements elimination, a Galerkin boundary node method (GBNM), is developed by combining the MLS approximation and a variational form of boundary integral equations. Boundary conditions in the GBNM can be applied directly and easily despite the MLS shape functions lack the delta function property. Besides, the GBNM keeps the symmetry and positive definiteness of the variational problems. Error analysis of the GBNM is established.

基于径向基函数插值的高精度差商及其在微分方程求解中的应用

冯仁忠²⁵²

Abstract: 利用具有零次代数精度的径向基函数插值的 Lagrange 形式给出被插函数在节点处的各阶差商 (简记 RBF-FD) 并特别对三等距节点的一阶和二阶 RBF 差商的逼近误差进行了分析, 分别给出使逼近阶达到最高阶的最佳参数值, 然后利用这些 RBF 差商公式分别求解了一阶常微分方程初值问题、两点边值问题和 Poisson 方程边值问题。由于在求解过程中巧妙地利用微分方程给出最佳参数, 使得所构造的高精度 RBF 差分格式的收敛阶是同节点模板的多项式差分 (简记 P-FD) 格式的 2 倍, 但计算时间几乎没有增加。

²⁵¹ 李小林, 重庆师范大学. Email: lxlmath@163.com

²⁵² 冯仁忠, 北京航空航天大学. Email: fengrz@buaa.edu.cn

Eulerian 网格下含内界面的定常扩散问题的一种有限体积格式的误差估计

彭洁, 舒适, 喻海元, 冯春生, 阚明先, 王刚华²⁵³

Abstract: The finite volume methods are frequently employed in the discretization of diffusion problems with interface. In this paper, we firstly present a vertex-centered MACH-like finite volume method for solving stationary diffusion problems with strong discontinuity and multiple material cells on the Eulerian quadrilateral grids. This method is motivated by Frese [No. AMRC-R-874, Mission Research Corp., Albuquerque, NM, 1987]. Then, the local truncation error and global error estimates of the degenerate five-point MACH-like scheme are derived by introducing some new techniques. Especially under some assumptions, we prove that this scheme can reach the asymptotic optimal error estimate $O(h^2 |\ln h|)$ in the maximum norm. Finally, numerical experiments verify theoretical results.

A monotone finite volume scheme for diffusion equations on general non-conforming meshes

Qi Zhang, Zhiqiang Sheng, Guangwei Yuan²⁵⁴

Abstract: A nonlinear monotone finite volume scheme on general non-conforming meshes for diffusion equations is introduced, which deals with discontinuous tensor coefficients rigorously. Since the expression of normal flux depends on auxiliary unknowns defined at cell-vertex including hanging nodes, we propose a new method to eliminate vertex-unknown by using primary unknowns at the centers of the cells sharing the vertex. Especially the unknowns defined on hanging nodes are eliminated by flux continuous conditions. The resulting scheme is monotone and preserves positivity of analytical solutions for strongly anisotropic and heterogeneous full tensor coefficient problems. Numerical results show that the convergent order of the monotone scheme by different methods of eliminating vertex unknowns will vary remarkably, and our new method can assure that it has almost second order accuracy and more accurate than some existing methods.

²⁵³ 彭洁, 湘潭大学. Email: xtu_pengjie@163.com

²⁵⁴ 张齐, 中国工程物理研究院研究生院. Email: zhanggogoqi@aliyun.com

分会场报告 6

S01-3 PDE 并行、快速算法研究进展

Nonlinearly Preconditioned Newton's Methods for PDEs

蔡小川²⁵⁵

Abstract: Inexact Newton is a popular technique for solving large sparse nonlinear system of equations. In this talk, we discuss some recently developed versions of preconditioned inexact Newton methods which are more robust than the classical version when the nonlinearities in the system are not balanced. The preconditioners are constructed using a combination of some domain decomposition methods and nonlinear elimination methods. We show numerically that the preconditioned inexact Newton methods perform well for solving some nonlinearly difficult problems, such as the hyperelasticity equation which is used to model the wall of human arteries.

基于格子 Boltzmann 模型的两相流数值模拟

黄记祖²⁵⁶

Abstract: 我们针对粗糙表面上大密度比的两相流问题，设计了有效的格子 Boltzmann 模型。采用 Chapman 展开的技术，可以从格子 Boltzmann 模型导出 Navier-Stokes 方程组和 Cahn-Hilliard 方程。为了描述流体在粗糙表面上的形为，我们采用非平衡外推的方法，实现 GNBC 边界条件。采用半隐式的方法离散求解格子 Boltzmann 模型，以实现大密度比的两相流问题的模拟。通过二维和三维的数值模拟，验证了模型的正确性和离散格式的稳定性。

²⁵⁵ 蔡小川, 中国科学院深圳先进技术研究院, University of Colorado Boulder. Email: cai@cs.colorado.edu

²⁵⁶ 黄记祖, 中国科学院数学与系统科学研究院科学与工程计算研究所. Email: huangjz@lsec.cc.ac.cn

Finite Volume Lattice Boltzmann Method for High Mach Compressible Flows on Unstructured Meshes

徐磊²⁵⁷

Abstract: A finite volume lattice Boltzmann equation (LBE) for high Mach compressible flows is developed. The proposed finite volume lattice Boltzmann method (FV-LBM) is grid-transparent which can be implemented on arbitrary unstructured meshes for effective and efficient treatment of complex geometries. A second order TVD scheme for the terms representing advection of the distribution function in physical space is adopted to discretize the LBE on cell-centered, arbitrary unstructured meshes. In this method, Qu and Shu's method is applied to simulate high Mach number compressible flows. The conventional Maxwellian distribution function is replaced by a circular function which is simple and satisfies all statistical relations to recover the compressible Navier-Stokes equations. Some test cases of compressible flows with strong shock waves are simulated to validate the proposed method. Excellent results are obtained.

S10-2 有限体积法理论及其应用

高次有限元方法的后处理算法

何文明²⁵⁸

Abstract: 我们将对有限元方法的超收敛性的研究做一个简单的回顾, 同时介绍报告人与合作者在高次有限元外推算法与插值后处理算法的研究工作。

Superconvergence of Immersed Finite Volume Methods for Interface Problems

曹外香²⁵⁹

Abstract: In this talk, we introduce a class of high order immersed finite volume methods (IFVM) for one dimensional interface problems. We show that the IFVM converge optimally in H^1 - and L^2 - norms. We also prove that the IFVM inherit all the desired superconvergence results from the standard finite volume methods. All theoretical results are confirmed by numerical experiments.

²⁵⁷ 徐磊, 上海大学. Email: leixushu@t.shu.edu.cn

²⁵⁸ 何文明, 温州大学.

²⁵⁹ 曹外香, 中山大学. Email: caowx5@mail.sysu.edu.cn

Cell-centered finite volume element methods for elliptic equations

刘玉洁²⁶⁰

Abstract: In this talk, we propose two cell-centered finite volume element (CCFVE) schemes for elliptic equations. Both of the two schemes obtain a finite element solution and an element-wisely-conserving flux simultaneously. It is shown that both the finite element solution and the numerical flux converge with optimal orders to the exact solution and flux, respectively. The theoretical results are verified by numerical test cases. To illustrate a motivation of this paper, a model of the two-phase flow in porous media has also been simulated. The numerical results match the physics and hence show that the locally conservative fluxes obtained by both CCFVE schemes perform well.

Generalized Finite Volume Methods for Elliptic Interface Problems

张庆辉²⁶¹

Abstract: In this talk, we present a generalized finite volume for elliptic interface problems. We will show that our methods converge with optimal order to the exact solution. Our theoretic findings are verified by several numerical experiments.

A Posteriori Error Estimates for Cell Functional Minimization Scheme Applied to Elliptic Equations

高志明²⁶²

Abstract: The major emphasis of this talk is the derivation of a posteriori error estimates for the cell functional minimization discrete scheme of second-order elliptic problem. A posteriori error estimates are reliable with respect to an energy-type error. The estimates are fully computable and locally efficient that they can serve as indicators for adaptive refinement and for the actual control of the error. Its performance is investigated numerically solving the elliptic equation on computational domains with different types of computational meshes and different shapes. It is found that the proposed adaptive cell functional minimization scheme offers a robust and accurate approach for solving second-order elliptic equations.

²⁶⁰ 刘玉洁, 中山大学. Email: liuyujie5@mail.sysu.edu.cn

²⁶¹ 张庆辉, 中山大学.

²⁶² 高志明, 北京应用物理与计算数学研究所.

S12-2 稀有事件及其鞍点问题的计算与应用

Numerical Study of the Effects of Surface Topography and Chemistry on the Wetting Transition Using the String method张亚楠²⁶³

Abstract: Droplets on a solid surface patterned with microstructures can exhibit the composite Cassie-Baxter (CB) state, or the wetted Wenzel state. The stability of the CB state is determined by the energy barrier separating it from the wetted state. In this work, we study the CB to Wenzel transition using the climbing string method [J. Chem. Phys. **126**, 164103 (2007), J. Chem. Phys. **138**, 134105 (2013)]. We compute the transition states and energy barriers for a three-dimensional droplet on patterned surfaces. The liquid-vapor coexistence is modeled using the mean field theory. Numerical results are obtained for surfaces patterned with straight pillars and nails, respectively. It is found that on both type of surfaces, wetting occurs via infiltration of the liquid in a single groove. The reentrant geometry of nails creates large energy barrier for the wetting of the solid surface compared to straight pillars. We also study the effect of surface chemistry, pillar height and inter-pillar spacing on the energy barrier, and compare it with nails.

The Application of the String method to the Dislocation Dynamics靳聪明²⁶⁴

Abstract: We present a numerical method to compute the transition rates including contributions from the potential energy and the entropy effect, of the thermally activated events in dislocation dynamics on the atomistic scale, based on the transition state theory and the string method. The method is applied to the migration of kinks in 30° partial dislocations in silicon. We also present atomistic simulation results on dislocation cross-slip in aluminum at zero temperature, with focus on the dependence of the transition paths and energy barriers on dislocation length and position. Multiple local minimum energy cross-slip paths have been found. A new mechanism with combination of the classical mechanisms has been identified.

²⁶³ 张亚楠, 苏州大学. Email: ynzhang@suda.edu.cn²⁶⁴ 靳聪明, 浙江理工大学. Email: jincm@lsec.cc.ac.cn

Recent Developments in Numerical Methods of Finding Saddle Points and its Applications in Materials

张磊²⁶⁵

Abstract: Nucleation is one of the most common physical phenomena in physical, chemical, biological and materials sciences. Due to the difficulties and challenges in making direct experimental observation, many computational methods have been developed to model and simulate various nucleation events. In my talk, I will provide a sampler of some newly developed numerical algorithms that are widely applicable to many nucleation and phase transformation problems. I first describe some recent progress on the design of efficient numerical methods for computing saddle points and minimum energy paths, and then illustrate their applications to the study of nucleation events associated with several different physical systems. Nucleation is a complex multiscale problem. Development of efficient numerical algorithms and modeling approaches is bringing new light to this challenging subject.

T02-2 流体力学中的数值计算

A phase-field fluid modeling and computation with interfacial profile correction term

Yibao Li (李义宝)²⁶⁶

Abstract: In this talk, we will present a new phase-field fluid modeling and computation with minimized Cahn–Hilliard dynamics. Using Cahn–Hilliard equation, the internal structure of the interface layer is determined by explicit smoothing of the flow discontinuities. This method greatly simplifies gridding, discretization and handling of topological changes. However, the original Cahn–Hilliard equation has intrinsic dynamics such as interface length minimization, i.e., the motion by minus the Laplacian of the mean curvature. When we apply the Cahn–Hilliard equation to model multiphase fluid flows, we want to minimize its interface length minimization property. Furthermore the surface tension formulation requires the interface of multiphase fluids be a hyperbolic tangent profile. Typically, under the advection of flow, the interfacial transition is not the hyperbolic tangent profile. That is, the interfacial transition is too compressed or sharpened. Even though the original Cahn–Hilliard dynamics conserves the total mass, the conservation of the enclosed area obtained by its interface can not remain. To overcome these shortcomings, we propose a modified Cahn–Hilliard equation with an interfacial profile correction term. Several numerical examples are presented to show the accuracy of the proposed method. The numerical results show that the proposed modified Cahn–Hilliard equation has better enclosed area preservation.

²⁶⁵ 张磊, 北京大学.

²⁶⁶ 李义宝, 西安交通大学. Email: yibaoli@xjtu.edu.cn

A Hybrid Smoothed Dissipative Particle Dynamics and Immersed Boundary method (SDPD-IBM) for Simulation of Red Blood Cells (RBCs) in Flows

叶挺²⁶⁷

Abstract: In biofluid flow systems, often the flow problems of fluids of complex structures, such as the flow of red blood cells (RBCs) through complex capillary vessels, need to be considered. The smoothed dissipative particle dynamics (SDPD), a particle-based method, is one of the easy and flexible methods to model such complex structure fluids. It couples the best features of the smoothed particle hydrodynamics (SPH) and dissipative particle dynamics (DPD), with parameters having specific physical meaning (coming from SPH discretization of the Navier-Stokes equations), combined with thermal fluctuations in a mesoscale simulation, in a similar manner to the DPD. On the other hand, the immersed boundary method (IBM), a preferred method for handling fluid-structure interaction problems, has also been widely used to handle the fluid-RBC interaction in RBC simulations. In this paper we aim to couple SDPD and IBM together to carry out the simulations of RBCs in complex flow problems. First, we develop the SDPD-IBM model in details, including the SDPD model for the evolving fluid flow, the RBC model for calculating RBC deformation force, the IBM for treating fluid-RBC interaction, and the solid boundary treatment model as well. We then conduct the verification and validation of the combined SDPD-IBM method. Finally, we demonstrate the capability of the SDPD-IBM method by simulating the flows of RBCs in rectangular, cylinder, curved, bifurcated and constricted tubes, respectively.

The Phase Transition Model for Heat-Shrinkable Thermo-Sensitive Hydrogels Based on Interaction Energy

Qiujin Peng, Hui Zhang and Zhengru Zhang²⁶⁸

Abstract: A biphasic mixture continuum mechanics model is derived for neutral heat-shrinkable thermo-sensitive hydrogels in this paper. The mixing free energy of the special mixture is recalculated based on the partition function of Bose system, and it evaluates the contribution of the hydrophilic, hydrophobic interaction and hydrogen bonding to the volume phase transition behaviors. The ideas of the Flory lattice theory and the UNIFAC group contribution method are employed to develop the expression of the mixing free energy. Numerical results demonstrate the reasonability of the new free energy expression.

²⁶⁷ 叶挺, 吉林大学. Email: yeting@jlu.edu.cn

²⁶⁸ 彭秋瑾, 中国人民大学. Email: pengqiujin@ruc.edu.cn

Error estimates for the decoupled, energy stable schemes for Cahn-Hilliard Phase-field models of two-phase incompressible flows

Zhen Xu, Xiaofeng Yang, Hui Zhang.²⁶⁹

Abstract: The aim of this paper is to carry out a rigorous error analysis of a decoupled energy stable schemes for solving the Cahn-Hilliard phase-field model of two-phase incompressible flows. The schemes combine the projection method, the explicit satbilizing decoupling technique, and linear stabilization/convex splitting method together. We derive optimal error estimates for these semi-discrete-in-time schemes based on the weak formulation thus the results can be carried over to any consistant finite-dimensional Galerkin type approximations since the proofs are all based on a variational formulation with all test functions in the same space as the space of the trial functions.

Characteristic block-centered finite difference method for simulating incompressible wormhole propagation

Xiaoli Li, Hongxing Rui²⁷⁰

Abstract: In this paper, the characteristic block-centered finite difference method is introduced and analyzed to solve the incompressible wormhole propagation. Error estimates for the pressure, velocity, porosity, concentration and its flux in different discrete norms are established rigorously and carefully on non-uniform grids. Finally, some numerical experiments are presented to show that the convergence rates are in agreement with the theoretical analysis.

Moving Staggered Mesh

赵刚²⁷¹

Abstract: Introducing a moving staggered mesh method and its development, and then we use the method to simulate incompressible flows.

²⁶⁹ 徐真, 北京师范大学. Email: xuzhenmath@163.com

²⁷⁰ 李晓丽, 山东大学. Email: xiaolisdu@163.com

²⁷¹ 赵刚, 中国科学院数学与系统科学研究院. Email: zhaog6@lsec.cc.ac.cn

T04-2 数值代数

An iterative scheme for identifying general H-tensor吕长青, 马昌凤²⁷²

Abstract: H-tensor plays an important role in identifying the positive (semi-)definiteness of even-order real symmetric tensor. In this paper, we propose an algorithm for identifying general H-tensor and prove the algorithm will terminate within finite iterative steps. At last, some numerical examples are provided to illustrate the efficiency and validity of methods we have proposed.

Ritz and harmonic Ritz values and the convergence of GMRESKui Du²⁷³

Abstract: We show that any GMRES residual norm history is possible with any prescribed admissible Ritz values, or any prescribed admissible harmonic Ritz values. The convergence of GMRES is also discussed.

Iterative solvers for elliptic problems with arbitrary anisotropy strengthsC. Yang, F. Deluzet²⁷⁴

Abstract: This paper is devoted to the introduction of iterative methods for the Asymptotic-Preserving (AP) resolution of anisotropic elliptic problems arising in magnetized plasma simulation. The methods investigated in this paper extend the precedent realizations, limited to the finite element framework, to finite difference discretizations. They also overcome the resolution of a Saddle point problem for which only sparse direct solvers have been successfully operated so far. Although very efficient for two dimensional computations, the cost of direct methods is considerable for real scale three dimensional problems hardly addressed in precedent achievements. This difficulty receives an appropriate answer in this paper, the new methods providing system matrices with a condition number uniformly bounded with respect to the anisotropy strength without the resolution of a Saddle point problem. An iterative resolution of the AP scheme is developed, offering a numerical cost comparable to the resolution of isotropic elliptic problems. This brings a leap forward in the computational efficiency of the method, conclusively outlined thanks to three dimensional serial computations carrying out tens of millions of unknowns.

²⁷² 吕长青, 枣庄学院. Email: 191590046@qq.com

²⁷³ 杜魁, 厦门大学. Email: kuidu@xmu.edu.cn

²⁷⁴ 杨畅, 哈尔滨工业大学. Email: yangchang@hit.edu.cn

一类五对角矩阵的特征值反问题及应用

吴静²⁷⁵

Abstract: 本文提出并解决了一类五对角矩阵的特征值反问题, 然后结合工程背景, 探讨了在梁系模型中的应用, 给出了两个算法和数值例子, 数值实验表明结论是正确的, 算法是有效, 为解决工程问题提供了一种方法和手段。

Effect Block Preconditioning for the Stationary MHD equations in 3D

李凌霄²⁷⁶

Abstract: In this report, we devise a parallel finite element iterative solver for the stationary magnetohydrodynamic equations. We adopt a mixed finite element method to solve the stationary magnetohydrodynamic equations where the velocity is approximated by H^1 -conforming finite elements and the magnetic field is approximated by H_{curl} -conforming edge elements. Based on preconditioning results for Navier-Stokes equations and Maxwell equations, an efficient preconditioner is proposed to accelerate the convergence of the Krylov subspace methods such as GMRES when solving the linearized problem of the discrete magnetohydrodynamic equations. With this solver, we simulate the Driven Cavity flow in 3D. The numerical experiments show that the preconditioning effect is perfect with respect to mesh refinement and effective for large Reynolds number, coupling number and magnetic Reynolds number. Moreover, the iterative solver is scalable provided the subproblem is effectively solved.

T08-2 自适应方法

Residual-Based A Posteriori Error Estimates for Symmetric Conforming Mixed Finite Elements for Linear Elasticity Problems

满红英²⁷⁷

Abstract: A posteriori error estimators for the symmetric mixed finite element methods for linear elasticity problems of Dirichlet and mixed boundary conditions are proposed. Stability and efficiency of the estimators are proved. Finally, we provide numerical examples to verify the theoretical results.

²⁷⁵ 吴静, 西安思源学院. Email: 656125381@qq.com

²⁷⁶ 李凌霄, 中国科学院数学与系统科学研究院. Email: lilingxiao@lsec.cc.ac.cn

²⁷⁷ 满红英, 北京理工大学. Email: manhy@lsec.cc.ac.cn

Residual based a posteriori error estimates for incompressible magnetohydrodynamics

Shipeng Mao, Weiying Zheng²⁷⁸

Abstract: We consider a mixed finite element method for the numerical discretization of a stationary incompressible magnetohydrodynamics problem in three dimensions with its velocity field is discretized using H^1 conforming elements and the magnetic field is approximated by curl-conforming Nédélec elements. Under the assumption that the original model has a unique solution pair, we derive a posteriori error estimates of the incompressible magnetohydrodynamic (MHD) equations with a sharp upper bound. Using these a posteriori error estimates, we construct an adaptive algorithm for computing the solution of 3D magnetohydrodynamics. Numerical experiments are carried out to show the performance of the adaptive finite element method.

自适应笛卡尔网格方法复杂几何模拟

刘剑明²⁷⁹

Abstract: 本文主要介绍自适应笛卡尔网格复杂几何问题的模拟方法。首先，我们将介绍基于虚拟单元的高精度间断有限元 (DG) 方法求解无粘 Euler 方程，并结合正保持方法求解复杂几何低密度或大马赫数问题。其次，为了能够使得自适应笛卡尔网格方法能够模拟高雷诺数粘性問題，我们也发展了一种基于壁面函数的虚拟单元方法。此外，在重叠网格框架下，我们也发展了一种混合自适应笛卡尔网格与非结构网格方法，并用于三维复杂外形的模拟。

A posteriori error analysis of nonconforming finite element methods for convection-diffusion problems

张蓓, 陈绍春, 赵纪坤, 毛士鹏²⁸⁰

Abstract: A unified framework is established for the a posteriori error analysis of nonconforming finite element approximations to convection-diffusion problems. Under some certain conditions, the theory assures the semi-robustness of residual error estimates in the usual energy norm and the robustness in a modified norm, and applies to several nonconforming finite elements, such as the Crouzeix-Raviart triangular element and the nonconforming rotated parallelogram element of Rannacher and Turek. Based on the general error decomposition in different norms, we show that the key ingredients of error estimation are the existence of a bounded linear operator with some elementary properties and the estimation on the consistency error related to the particular numerical scheme. The numerical results are presented to illustrate the practical behavior of the error estimator and check the theoretical predictions.

²⁷⁸ 毛士鹏, 中科院计算数学所. Email: maosp@lsec.cc.ac.cn

²⁷⁹ 刘剑明, 江苏师范大学. Email: jmliu@jsnu.edu.cn

²⁸⁰ 张蓓, 郑州大学. Email: zhangbeizhu@126.com

T09-5 分数阶方程

分数阶偏微分方程的快速算法

王宏²⁸¹

Abstract: Fractional partial differential equations (FPDEs) are emerging as a powerful tool for modeling challenging phenomena including anomalous diffusive transport processes, and long range time memory or spatial interactions. Computationally, the numerical methods for these problems often generate dense coefficient matrices for which traditional direct solvers were used that have a computational complexity of $O(N^3)$ per time step and memory requirement of $O(N^2)$ where N is the number of unknowns. This makes numerical simulation of these nonlocal models computationally very expensive. We will go over the development of fast numerical methods for these problems, by exploring the structure of the coefficient matrices. These methods have approximately linear computational complexity per time step and optimal memory requirement.

Numerical solution of evolutionary integral equations with completely monotonic kernel by Runge-Kutta convolution quadrature

Da Xu²⁸²

Abstract: We study the numerical solutions of the initial boundary value problems for the Volterra type evolutionary integral equations, in which the integral operator is a convolution product of a completely monotonic kernel and a positive definite operator, such as a elliptic partial differential operator. The equation is discretized in time by the Runge-Kutta convolution quadrature. Error estimates are derived and numerical experiments reported.

Muntz Spectral Methods with Applications to Some Singular Problems

Dianming Hou, Chuanju Xu²⁸³

Abstract: In this talk we will present a fractional spectral method for a class of equations with non-smooth solutions. The proposed method makes new use of the classical fractional polynomials, also known as Muntz polynomials. We will show how to construct efficient fractional spectral methods for some integro-differential equations which can achieve spectral accuracy for solutions with limited regularity. A detailed convergence analysis will be provided. The potential application of this method covers a large number of problems, including integro-differential equations with weakly singular kernels, fractional differential equations, and so on.

²⁸¹ 王宏, 南卡罗来纳大学 / 山东大学. Email: 58267876@qq.com

²⁸² 徐大, 湖南师范大学. Email: daxu@hunnu.edu.cn

²⁸³ 许传炬, 厦门大学. Email: cjxu@xmu.edu.cn

Convergence analysis of a multigrid method for the nonlocal model

Minghua Chen²⁸⁴

Abstract: Recently, nonlocal models attract the wide interest of scientists. They mainly come from two applied scientific fields: peridynamics and anomalous diffusion. Even though the matrices of the algebraic equation corresponding the nonlocal models are usually Toeplitz (denote a_0 as the principal diagonal element, a_1 as the trailing diagonal element, etc). There are still some differences for the models in these two fields. For the model of anomalous diffusion, a_0/a_1 is uniformly bounded; most of the time, a_0/a_1 of the model for peridynamics is unbounded as the stepsize h tends to zero. Based on the uniform boundedness of a_0/a_1 , the convergence of the two-grid method is well established [Chan, Chang, and Sun, SIAM J. Sci. Comput., 19 (1998), pp. 516–529; Pang and Sun, J. Comput. Phys., 231 (2012), pp. 693–703; Chen, Wang, Cheng, and Deng, BIT, 54 (2014), pp. 623–647]. This paper provides the detailed proof of the convergence of the two-grid method for the nonlocal model of peridynamics. Some special cases of the full multigrid and the V-cycle multigrid are also discussed. The numerical experiments are performed to verify the convergence.

T12-2 移动网格和无网格及有限体积法

Finite volume element method for nonlinear elliptic and parabolic optimal control problems

Zuliang Lu²⁸⁵

Abstract: In this work, we study a priori error estimates for the finite volume element approximation of nonlinear elliptic and parabolic optimal control problem. The schemes use discretizations base on a finite volume method, for the variational inequality, we use the method of the variational discretization concept to obtain the control. Under some reasonable assumptions, we obtain some optimal order error estimates. Some numerical experiments are presented to test the theoretical results.

²⁸⁴ 陈明华, 兰州大学. Email: chenmh@lzu.edu.cn

²⁸⁵ 鲁祖亮, 重庆三峡学院. Email: zulianglux@126.com

A moving mesh finite difference method for equilibrium radiation diffusion equations

Xiaobo Yang, Weizhang Huang and Jianxian Qiu²⁸⁶

Abstract: An efficient moving mesh finite difference method is developed for the numerical solution of equilibrium radiation diffusion equations in two dimensions. The method is based on the moving mesh partial differential equation approach and moves the mesh continuously in time using a system of meshing partial differential equations. The mesh adaptation is controlled through a Hessian-based monitor function and the so-called equidistribution and alignment principles. Several challenging issues in the numerical solution are addressed. Particularly, the radiation diffusion coefficient depends on the energy density highly nonlinearly. This nonlinearity is treated using a predictor-corrector and lagged diffusion strategy. Moreover, the nonnegativity of the energy density is maintained using a cutoff method which has been known in literature to retain the accuracy and convergence order of finite difference approximation for parabolic equations. Numerical examples with multi-material, multiple spot concentration situations are presented. Numerical results show that the method works well for radiation diffusion equations and can produce numerical solutions of good accuracy. It is also shown that a two-level mesh movement strategy can significantly improve the efficiency of the computation.

Fourier finite volume element method for Dirichlet boundary control problems governed by parabolic PDEs

Tengjin Zhao(赵腾进), Zhiyue Zhang(张志跃)²⁸⁷

Abstract: We study the optimal control problem governed by a parabolic partial differential equation with Dirichlet boundary conditions. We propose a Fourier finite volume element method based on Galerkin variational formulation for the Dirichlet boundary parabolic equation on an annular domain. We apply the Fourier expansion in the azimuthal direction and use the finite volume element method in the radial direction respectively. Finally, numerical experiments demonstrate the proposed method is effective for sloving this problem.

²⁸⁶ 杨晓波, 中国矿业大学. Email: xwindyb@126.com

²⁸⁷ 赵腾进, 南京师范大学. Email: 584743381@qq.com

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