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Summer, 2006

Greeting

Hiroshi Fujita （藤田　宏）

As the honorary organizer, I wish to welcome you to the First China-Japan-Korea Joint Conference on Numerical Mathematics, and wish you to enjoy scientific exchanges and cool summer in Sapporo. My gratitude goes to coordinators from the three countries, Professors Zhong-Ci Shi, Hisashi Okamoto, Dongwoo Sheen, who have planned and materialized this important meeting, and also goes to local organizers, scientific advisors and all the other members who have helped the coordinators.

The three countries are geographically neighbors and are culturally linked since ancient years. For instance, more than thousand years ago, Chinese characters (letters) came to Japan from China (along with Buddhism) via Korea, which was followed by import of general Chinese culture and by import of various Korean craftsmanship, while Japan served as the first runner to introduce Western science and technology into East Asia for several decades since she opened her door to the outside about 150 years ago. From this point of view, I can see that friendly collaboration of the three countries through the CJK conference can be and will be successfully achieved.

It would be also my duty to refer to a forerunner of the CJK conference, i.e. China-Japan Joint Seminar on Numerical Mathematics, a series of seven conferences held every two years since 1992, which contributed much to promote scientific collaboration and to confirm friendship between Chinese and Japanese researchers in the relevant fields. For it, Prof. Zhong-Ci Shi was the standing coordinator from Chinese side, while the rotating task of Japanese coordinator was taken by Professors Teruo Ushijima, Masatake Mori, Hideo Kawarada, Makoto Natori and Hisashi Okamoto. I can also recollect preliminary but earnest discussions toward the CJ collaboration which were made in 1981 with Chinese leaders including Professors Su Buchin, Gu Chaohao and Feng Kang, when I visited China for the first time.

As to the global aim of science, it is now claimed (e.g. by ICSU) that science in this century must be ‘science for the human society’ instead of traditional ‘science for science’. In nature, Numerical Mathematics is directly connected with enforcement of human understanding of natural and social phenomena, and with creation of powerful methods to solve serious problems met by humankind. In this connection, I dare say that researchers of the CJK countries share a good point in doing Numerical Mathematics for the above-mentioned purposes; that is Wisdom in the East.

Thus I wish and believe success of the CJK conference.

Program

August 3, 2006 (Thursday)

9:15-9:55 Opening Session

10:00-10:40 Zhong-Ci Shi (Chinese Academy of Sciences)
石　鐘慈（中国科学院）
Some Aspects of Finite Element Approximation for Reissner-Mindlin Plates

11:00-11:40 Masahisa Tabata (Kyushu University)
田端　正久（九州大学）
Energy-Stable Finite Element Schemes for Multiphase Flow Problems

11:45-12:25 Hongxing Rui (Shandong University)
芮　洪興（山東大学）
Split Least-squares Mixed Element Methods

14:00-14:40 Byeong-Chun Shin (Chonnam National University)
辛　炳春（全南大学）
Least-squares Mixed Methods Using $RT_0 \times P_1$ Space for Elliptic Boundary Value Problems

14:45-15:05 Qing Fang (Yamagata University)
方　青（山形大学）
Convergence of Finite Difference Methods for Poisson-Type Equations with Singular Solutions

15:10-15:30 Shigetoshi Yazaki (University of Miyazaki)
矢崎　成俊（宮崎大学）
Numerical Simulation of an Area-Preseving Crystalline Curvature Flow

16:00-16:20 Tomohiro Sogabe (Nagoya University)
曽我部　知広（名古屋大学）
CRS: A Fast Algorithm Based on Bi-CR for Solving Nonsymmetric Linear Systems

16:25-17:05 Dongyang Shi (Zhengzhou University)
石　東洋（鄭州大学）
Convergence Analysis of Nonconforming Incomplete Biquadratic Plate Element on Anisotropic Meshes

17:10-17:30 Deng Li (University of Kentucky／ケンタッキー大学)
DDDAS Approaches to Wildland Fire Modeling

18:30-20:30 Party

August 4, 2006 (Friday)

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申　東雨（ソウル大学）
Analysis of Conforming and Nonconforming Finite Element Methods in Wave Propagation

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湯　濤（香港浸会大学）
Moving Mesh Methods for Singular Problems Using Perturbed Harmonic Mappings

11:00-11:40 Takashi Kako (The University of Electro-Communications)
加古　隆（電気通信大学）
Numerical Methods for Wave Propagation Problem Applied to Voice Generation Simulation

11:45-12:25 Yu-Jiang Wu (Lanzhou University)
伍　渝江（蘭州大学）
Semi-Implicit Schemes with Multilevel Wavelet-like Incremental Unkowns for a Reaction-Diffusion Equation

14:00-16:00 Poster Session & Group Photo

16:00-16:20 Awarding Ceremony

16:25-17:05 Weiwei Sun (City University of Hong Kong／香港城市大学)
Mathematical Modeling for Moisture Transport in Fibrous Materials and Applications

17:10-17:30 Takuya Tsuchiya (Ehime University)
土屋　卓也（愛媛大学）
Conformal Mappings to Exterior Jordan Domains and their Finite Element Approximation

August 5, 2006 (Saturday)

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松尾　宇泰（東京大学）
A conservative Galerkin Scheme for the KdV Equation

10:00-10:40 Youngmok Jeon (Ajou University)
全　永穆（亜州大学）
The Cell Boundary Element Methods

11:00-11:40 Yoshimasa Nakamura (Kyoto Univeristy)
中村　佳正（京都大学）
New Singular Value Decomposition Algorithm with High Performance

11:45-12:25 Linzhang Lu (Xiamen University／廈門大学)
A New Look at Restarted GMRES Method

14:00-14:40 Tetsuya Sakurai (University of Tsukuba)
櫻井　鉄也（筑波大学）
A Rayleigh-Ritz Type Method for Large-Scale Generalized Eigenvalue Problems

14:45-15:25 Donghui Li (Hunan University)
李　董輝（湖南大学）
Descent Nonlinear Congugate Gradient Methods for Optimization

16:00-16:40 Zhong-Zhi Bai (Chinese Academy of Sciences／中国科学院)
Iterative Splitting Methods for Nonsymmetric Algebraic Riccati Equations

August 6, 2006 (Sunday)

9:15-9:55 Zhiming Chen (Chinese Academy of Sciences／中国科学院)
A Posteriori Error Analysis and Adaptive Methods for Partial Differential Equations

10:00-10:40 Seokchan Kim (Changwon National University／昌原大学)
The Finite Element Methods Dealing with Domain Singularities

11:00-11:40 Hiroshi Fujiwara (Kyoto University)
藤原　宏志（京都大学）
High-Accurate Numerical Computation with Multiple-precision Arithmetic and Spectral Method

11:45-12:25 Chang-Ock Lee (KAIST)
李　昌沃（韓国科学技術院）
A Neumann-Dirichlet Preconditioner for a Feti-DP Formulation with Mortar Methods

14:00-14:40 Mitsuhiro T. Nakao (Kyushu University)
中尾　充宏（九州大学）
Numerical Verification Methods of Bifurcating Solutions for Two- and Three-Dimensional Rayleigh-Bénard Problems

August 7, 2006 (Monday)

Excursion to Hokkaido's volcanic area（登別　地獄谷）

Contents

Some Aspects of Finite Element Approximation for Reissner-Mindlin Plates

Zhong-Ci SHI and Pingbing MING

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Abstract
======

Reissner-Mindlin plate model is one of the most commonly used models of a moderately think to thin linearly elastic plate. However, a direct and seemingly reasonable finite element discretization usually yields very poor results which is usually referred to LOCKING phenomenon. In the past two decades, many efforts have been devoted to the design of locking free finite elements to resolve this model. However, most of these work focus on triangular and rectangular elements, the latter may be easily extended to parallelograms, but very few on quadrilaterals.

In this talk we will give an overview for the recent development of some low order quadrilateral elements and present our new results.

Energy-Stable Finite Element Schemes for Multiphase Flow Problems

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Abstract

We study numerical analysis of multiphase flow problems by finite element methods. Let Ω be a bounded domain in $\mathbf{R}^2$ and T be a positive number. Suppose that Ω is occupied by two immiscible fluids with densities ρ_k and viscosities μ_k, $k = 1, 2$, governed by the unsteady Navier-Stokes equations

$$\begin{aligned} \rho_k \left\{ \frac{\partial u}{\partial t} + (u \cdot \nabla) u \right\} - \nabla(2\mu_k D(u)) + \nabla p &= \rho_k f, \\ \nabla \cdot u &= 0, \end{aligned}$$

in each domain

$$Q_k(T) \equiv \{(x, t);\ x \in \Omega_k(t),\ 0 < t < T\},$$

where f is a given function, $D(u)$ is the strain-rate tensor, and $\Omega_k(t)$ are domains to be found. On the interface $\partial\Omega_1(t) \cap \partial\Omega_2(t)$, $t \in (0, T)$, interface conditions

$$[u] = 0, \qquad [\sigma(\mu, u, p)n] = \gamma_0 \kappa n$$

are imposed, where $[\cdot]$ means the difference of the values approached from both sides to the interface, κ is the curvature of the interface, γ_0 is the coefficient of the interfacial tension, n is the unit normal vector, and σ is the stress tensor. We impose slip boundary conditions on the boundary of Ω, and initial conditions on u. Initial fluids domains $\Omega_k(0)$, $k = 1, 2$, are given.

We present finite element schemes for this problem, discuss the stability, and apply them to rising bubble problems. The following figure shows a numerical simulation of a bubble movement in a fluid.

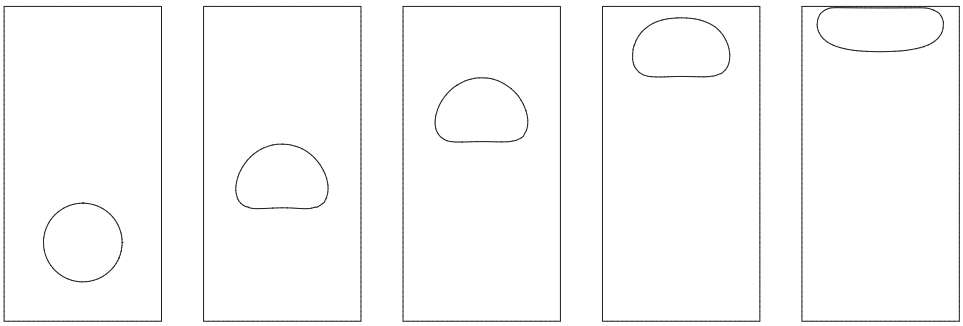

Figure 1: $\Omega_1(t)$ at $t = 0.0, 2.5, 5.0, 7.5, 10.0$ ($\gamma_0 = 2.0$)

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Split Least-squares Mixed Element Methods

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Abstract. In this paper, we propose some least-squares mixed finite element procedures for reaction-diffusion equations and parabolic equations based on the first-order system. By select the functional properly each proposed procedure can be splitted into two independent symmetric positive definite sub-procedures, one of which is for the primary unknown variable u and the other of which is for the expanded flux unknown variable σ. Optimal order error error estimates are developed. Finally we give some numerical examples which are in a good agreement with the theoretical analysis.

*This work is supported by the National Natural Science Foundation of China Grant No. 10471079 and the Research Fund for Doctoral Program of High Education by State Education Ministry of China.

†This is a cooperation with Sang Dong Kim and Seokchan Kim and is also supported by the Korea Research Foundation under contract number KRF-2002-070-C00014.

Least-squares mixed methods using $RT_0 \times P_1$ space for elliptic boundary value problems

Byeong-Chun Shin*

Abstract

We first review the first-order system least-squares (FOSLS) approaches for elliptic boundary value problems. The least-squares functionals are defined by summing L^2-norm or H^{-1}-norm of residual equations. Also we review the first-order system LL^* (FOSLL*) developed using adjoint equations in recent for elliptic problems. Such an adjoint approach employs the developed extended first-order operator and its corresponding adjoint first-order operator for a given second-order elliptic boundary value problem. Also the method uses H^1-norm equivalent least squares functional where the finite elements methods using the product piecewise linear function space $(P_1)^4$ in $2D$ are used for approximations including a scalar variable, a vector variable and one more auxiliary scalar variable.

In this talk, our main approach is using the lowest Raviart-Thomas element space, RT_0, for vector variable and conforming piecewise linear space, P_1, for scalar variable. Using these space we also develop FOSLL* using adjoint approach to solve general elliptic problems having corner singularities or discontinuous coefficients. Our least-squares functional is equivalent to $H(div) \times H^1$-norm of the product space $RT_0 \times P_1$.

1 Introduction

Let Ω be a bounded, open, simply connected domain in $\mathbb{R}^d$, $d = 2, 3$. Consider the following elliptic equation

$$\left\{ \begin{array}{rcl} \nabla \cdot A\nabla p - \mathbf{b} \cdot \nabla p - c\,p &=& f, \quad \text{in } \Omega, \\ p &=& 0, \quad \text{on } \Gamma_D, \\ \mathbf{n} \cdot A\nabla p &=& 0, \quad \text{on } \Gamma_N, \end{array} \right. \tag{1.1}$$

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where $\partial\Omega = \Gamma_D \cup \Gamma_N$ denotes the boundary of Ω, $f \in L^2(\Omega)$, $0 \le c \in L^\infty(\Omega)$, $\mathbf{b} \in L^\infty(\Omega) \cap H(\mathrm{div})$, and A is a $d \times d$ uniformly symmetric positive definite matrix of $L^\infty(\Omega)$-functions, i.e.,

$$0 < \lambda\, \boldsymbol{\xi}^t \boldsymbol{\xi} \le \boldsymbol{\xi}^t A(x,y) \boldsymbol{\xi} \le \Lambda\, \boldsymbol{\xi}^t \boldsymbol{\xi} < \infty \tag{1.2}$$

for all $\boldsymbol{\xi} \in \mathbb{R}^2$ and $\mathbf{x} \in \Omega$, and $\mathbf{n}$ is the outward unit vector normal to the boundary.

We assume that (1.1) has the unique solution in $H^1(\Omega)$ and the adjoint problem

$$\left\{ \begin{array}{rcll} \nabla \cdot A\nabla p + \nabla \cdot (\mathbf{b}p) - c\,p & = & f, & \text{in } \Omega, \\ p & = & 0, & \text{on } \Gamma_D, \\ \mathbf{n} \cdot (A\nabla p + \mathbf{b}p) & = & 0, & \text{on } \Gamma_N \end{array} \right. \tag{1.3}$$

also has the unique solution in $H^1(\Omega)$.

Let $\mathbf{u}$ be a new vector variable such as

$$\mathbf{u} = A^{\frac{1}{2}} \nabla p.$$

Then the equation (1.1) becomes

$$L(\mathbf{u}, p) := \left\{ \begin{array}{rcll} A^{-1/2}\mathbf{u} - \nabla p & = & \mathbf{0}, & \text{in} \quad \Omega, \\ \nabla \cdot A^{1/2}\mathbf{u} - \mathbf{b} \cdot A^{-1/2}\mathbf{u} - c\,p & = & f, & \text{in} \quad \Omega \end{array} \right.$$

with boundary conditions

$$\begin{array}{rcll} \mathbf{n} \cdot A^{1/2}\mathbf{u} & = & 0, & \text{on} \quad \Gamma_N, \\ p & = & 0, & \text{on} \quad \Gamma_D, \end{array}$$

that is, the differential operator is given by

$$L(\mathbf{u}, p) := \begin{bmatrix} A^{-1/2} & -\nabla \\ \nabla \cdot A^{1/2} - \mathbf{b} \cdot A^{-1/2} & -c \end{bmatrix} \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix}.$$

The domain $\mathcal{D}(L)$ of L is

$$\mathcal{D}(L) = H_N(\mathrm{div}\, A^{1/2}) \times H_D^1(\Omega),$$

which is a Hilbert space under the norm

$$\|(\mathbf{v}, q)\|^2_{\mathcal{D}(L)} := \|\mathbf{v}\|^2_{H(\mathrm{div}\, A^{1/2})} + \|q\|_1^2.$$

The FOSLL* approach is to approximate the solution $(\bar{\mathbf{u}}, \bar{p})$ of the corresponding dual problem

$$L^*(\bar{\mathbf{u}}, \bar{p}) \quad = \quad (A^{1/2}\nabla p, p)^t = (\mathbf{u}, p)^t, \quad \text{in} \quad \Omega,$$

where

$$L^*(\bar{\mathbf{u}}, \bar{p}) := \begin{bmatrix} A^{-1/2} & -A^{1/2}\nabla - A^{-1/2}\mathbf{b} \\ \nabla\cdot & -c \end{bmatrix} \begin{pmatrix} \bar{\mathbf{u}} \\ \bar{p} \end{pmatrix}$$

with boundary conditions

$$\begin{cases} \mathbf{n}\cdot\bar{\mathbf{u}} &= 0 \quad \text{on} \quad \Gamma_N, \\ \bar{p} &= 0 \quad \text{on} \quad \Gamma_D. \end{cases}$$

The domain $\mathcal{D}(L^*)$ of L^* is

$$\mathcal{D}(L^*) = H_N(\text{div}) \times H_D^1(\Omega).$$

which is a Hilbert space under the norm

$$\|(\bar{\mathbf{v}}, \bar{q})\|^2_{\mathcal{D}(L^*)} := \|\bar{\mathbf{v}}\|^2_{H(\text{div})} + \|\bar{q}\|^2_1.$$

The primal problem is equivalent to minimizing the following functional

$$\begin{aligned} G(\mathbf{v}, q) &= \|L(\bar{\mathbf{v}}, \bar{q}) - (\mathbf{0}, f)^t\|^2 \\ &= \|A^{-1/2}\mathbf{v} - \nabla q\|^2 + \|\nabla\cdot A^{1/2}\mathbf{v} - \mathbf{b}\cdot A^{-1/2}\mathbf{v} - c\,q - f\|^2 \end{aligned}$$

over $(\mathbf{v}, q) \in \mathcal{D}(L)$. Then the corresponding variational problem is to find $(\mathbf{u}, q)^t \in \mathcal{D}(L)$ such that

$$\mathcal{A}\Big((\mathbf{u}, p), (\mathbf{v}, q)\Big) = \mathcal{F}\Big((\mathbf{v}, q)\Big) \quad \forall\, (\mathbf{v}, q) \in \mathcal{D}(L),$$

where the bilinear form $\mathcal{A}(\cdot;\cdot)$ is given by

$$\begin{aligned} \mathcal{A}\Big((\mathbf{u}, p),(\mathbf{v}, q)\Big) &= \Big\langle L(\mathbf{u}, p),\, L(\mathbf{v}, q)\Big\rangle \\ &= \Big\langle A^{-1/2}\mathbf{u} - \nabla p,\, A^{-1/2}\mathbf{v} - \nabla q\Big\rangle \\ &\quad + \Big\langle \nabla\cdot A^{1/2}\mathbf{u} - \mathbf{b}\cdot A^{-1/2}\mathbf{u} - c\,p,\, \nabla\cdot A^{1/2}\mathbf{v} - \mathbf{b}\cdot A^{-1/2}\mathbf{v} - c\,q\Big\rangle \end{aligned}$$

and the linear form $\mathcal{F}(\cdot)$ is given by

$$\mathcal{F}\Big((\mathbf{v}, q)\Big) = \Big\langle (\mathbf{0}, f)^t,\, L(\mathbf{v}, q)\Big\rangle = \Big\langle f,\, \nabla\cdot A^{1/2}\mathbf{v} - \mathbf{b}\cdot A^{-1/2}\mathbf{v} - c\,q\Big\rangle.$$

Furthermore, the dual problem is equivalent to minimizing the dual functional

$$G^*(\bar{\mathbf{v}}, \bar{q}) = \|L^*(\bar{\mathbf{v}}, \bar{q}) - (\mathbf{u}, p)^t\|^2$$

over $(\bar{\mathbf{v}}, \bar{q}) \in \mathcal{D}(L^*)$. The corresponding variational problem is to find $(\bar{\mathbf{u}}, \bar{q})^t \in \mathcal{D}(L^*)$ such that

$$\mathcal{A}^*\Big((\bar{\mathbf{u}}, \bar{p}), (\bar{\mathbf{v}}, \bar{q})\Big) = \mathcal{F}^*\Big((\bar{\mathbf{v}}, \bar{q})\Big) \quad \forall\, (\bar{\mathbf{v}}, \bar{q}) \in \mathcal{D}(L^*),$$

where the bilinear form $\mathcal{A}^*(\cdot;\cdot)$ is given by

$$\begin{aligned}\mathcal{A}^*\Big((\bar{\mathbf{u}},\bar{p}),(\bar{\mathbf{v}},\bar{q})\Big) &= \Big\langle L^*(\bar{\mathbf{u}},\bar{p}),\, L^*(\bar{\mathbf{v}},\bar{q})\Big\rangle \\ &= \Big\langle A^{-1/2}\bar{\mathbf{u}} - A^{1/2}\nabla\bar{p} - A^{-1/2}\mathbf{b}\,\bar{p},\, A^{-1/2}\bar{\mathbf{v}} - A^{1/2}\nabla\bar{q} - A^{-1/2}\mathbf{b}\,\bar{q}\Big\rangle \\ &\quad + \Big\langle \nabla\cdot\bar{\mathbf{u}} - c\bar{p},\, \nabla\cdot\bar{\mathbf{v}} - c\bar{q}\Big\rangle\end{aligned}$$

and the linear form $\mathcal{F}^*(\cdot)$ is given by

$$\mathcal{F}^*\Big((\bar{\mathbf{v}},\bar{q})\Big) = \Big\langle (\mathbf{u},p)^t,\, L^*(\bar{\mathbf{v}},\bar{q})\Big\rangle = \Big\langle (\mathbf{0},f)^t,\, (\bar{\mathbf{v}},\bar{q})\Big\rangle = \Big\langle f,\, \bar{q}\Big\rangle,$$

where the unknown primal variable $(\mathbf{u},p)$ was eliminated by property of the dual operator L^*.

In this paper we show the well-posedness for the operator L and L^* and error estimates using the Raviart-Thomas space RT_0 for vector variable and continuous piecewise linear function space P_1 for scalar variable, and then we present several numerical experiments for elliptic problem having discontinuous coefficients or corner singularities.

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Convergence of Finite Difference Methods for Poisson-Type Equations with Singular Solutions

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In this paper, we are concerned with the following Dirichlet boundary value problem of elliptic equations on a disk.

$$-\Delta u + c_1(x,y)u = f_1(x,y) \quad \text{in } \Omega_1, \tag{1}$$

$$u = g_1(x,y) \quad \text{on } \Gamma_1 = \partial\Omega_1, \tag{2}$$

where $c_1(x,y) \geq 0$, $\Omega_1 = \{(x,y) \mid x^2+y^2 < R^2\}$ $(R > 0)$.

By using ploar coordinates, the above problem can be rewritten as

$$-\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}\right] + c(r,\theta)u = f(r,\theta) \qquad \text{in } \Omega, \tag{3}$$

$$u(R,\theta) = g(\theta) \qquad \text{on } \Gamma = \partial\Omega, \tag{4}$$

where $\Omega = \{(r,\theta) \mid 0 < r < R, 0 \leq \theta < 2\pi\}$ and $\Gamma = \{(R,\theta) \mid 0 \leq \theta < 2\pi\}$.

Let

$$\varphi(t) = R - (R-t)^{p+1}/R^p \quad (0 \leq t \leq 1),$$

which satisfies $\varphi(0) = 0, \varphi(R) = R$. We take the following partititon of Ω and apply Swartztrauber-Sweet method to (3)–(4).

$$h = \frac{R}{m+1}, \quad t_i = ih, \quad r_i = \varphi(t_i), \quad i = 0,1,2,\cdots,m+1$$

$$r_{i+1/2} = (r_i + r_{i+1})/2, \quad i = 0,1,2,\cdots,m$$

$$h_i = r_i - r_{i-1}, \quad i = 1,2,\cdots,m+1$$

$$k = \frac{2\pi}{n}, \quad \theta_j = jk, \quad j = 0,1,2,\cdots,n$$

$$-\left[\frac{1}{r_i}\left\{\frac{r_{i+1/2}(U_{i+1,j}-U_{i,j})}{h_{i+1}} - \frac{r_{i-1/2}(U_{i,j}-U_{i-1,j})}{h_i}\right\}\Big/\left(\frac{h_i+h_{i+1}}{2}\right)\right.$$
$$\left. + \frac{1}{r_i^2k^2}(U_{i,j+1} - 2U_{i,j} + U_{i,j-1})\right] + c_{i,j}U_{i,j} = f_{i,j},$$
$$i = 1,2,\cdots,m;\ j = 0,1,2,\cdots,n-1$$

$$\frac{4}{h_1^2}\left[U_{0,0} - \frac{1}{n}\sum_{j=0}^{n-1} U_{1,j}\right] + c_{0,0}U_{0,0} = f_{0,0},$$

$$U_{i,n} = U_{i,0} \quad U_{i,-1} = U_{i,n-1}, \quad i = 0, 1, 2, \cdots, m+1$$

$$U_{0,j} = U_{0,0}, \quad U_{m+1,j} = g_j, \quad j = 0, 1, 2, \cdots, n$$

We consider the approximate solutions when exact solutions of (3)–(4) have some singular properies whose derivatives go to infinity at the boundary. Convergence analysis results and numerical examples to illustrate will be given in the talk.

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Numerical simulation of an area-preserving crystalline curvature flow*

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1. Introduction

In this talk, a numerical scheme and simulation of an area-preserving crystalline cuvature flow for plane curves will be presented. A crystalline cuvature flow is motion of polygonal curves, and can be regarded as a discrete version of a weighted curvature flow, especially from a numerical point of view. A weighted curvature flow follows from the gradient flow for a total amount, say $\mathcal{F}$, of smooth interfacial energies defined on a smooth curve. However, some materials have non-smooth interfacial energy including crystalline energy. For such an energy, we can not calculate the gradient flow of $\mathcal{F}$ in the classical sense. In around 1990, for a crystalline energy, J. E. Taylor [6] and S. Angenent and M. E. Gurtin [1] proposed the following formulation: motion of a special class of curves —admissible polygonal curves— by crystalline curvature. We refer the reader to a survey [3].

Polygonal curves. Let $\mathcal{P}$ be a simple closed N-sided polygonal curve in the plane $\mathbb{R}^2$, and label the position vector of vertices $\boldsymbol{p}_i$ $(i = 1, 2, \ldots, N)$ in an anticlockwise order: $\mathcal{P} = \bigcup_{i=1}^{N} \mathcal{S}_i$ where $\mathcal{S}_i = [\boldsymbol{p}_i, \boldsymbol{p}_{i+1}]$ is the i-th edge $(\boldsymbol{p}_{N+1} = \boldsymbol{p}_1)$. The length of $\mathcal{S}_i$ is $d_i = |\boldsymbol{p}_{i+1} - \boldsymbol{p}_i|$, and then the i-th unit tangent vector is $\boldsymbol{t}_i = (\boldsymbol{p}_{i+1} - \boldsymbol{p}_i)/d_i$ and the i-th unit outward normal vector is $\boldsymbol{n}_i = -\boldsymbol{t}_i^{\perp}$, where $(a, b)^{\perp} = (-b, a)$. Put $\mathcal{N} = \{\boldsymbol{n}_1, \boldsymbol{n}_2, \ldots, \boldsymbol{n}_N\}$. Let θ_i be the exterior normal angle of $\mathcal{S}_i$. Then $\boldsymbol{n}_i = \boldsymbol{n}(\theta_i)$ and $\boldsymbol{t}_i = \boldsymbol{t}(\theta_i)$ hold, where $\boldsymbol{n}(\theta) = (\cos\theta, \sin\theta)$ and $\boldsymbol{t}(\theta) = (-\sin\theta, \cos\theta)$. We define the i-th hight function $h_i = \langle \boldsymbol{p}_i, \boldsymbol{n}_i \rangle = \langle \boldsymbol{p}_{i+1}, \boldsymbol{n}_i \rangle$. By using N-tuple $h = (h_1, h_2, \ldots, h_N)$, d_i is described as follows:

$$d_i[h] = -(\cot\vartheta_i + \cot\vartheta_{i+1})h_i + h_{i-1}\operatorname{cosec}\vartheta_i + h_{i+1}\operatorname{cosec}\vartheta_{i+1}, \tag{1}$$

where $\vartheta_i = \theta_i - \theta_{i-1}$ for $i = 1, 2, \ldots, N$. Note that $0 < |\vartheta_i| < \pi$ holds for all i.

Crystalline energy. We assume the interfacial energy density $\gamma : \mathbb{R}^2 \to \mathbb{R}_+$ is convex and satisfies $\gamma(\lambda \boldsymbol{x}) = \lambda\gamma(\boldsymbol{x})$ for all $\lambda \geq 0$ and $\boldsymbol{x} \in \mathbb{R}^2$. If the Frank diagram $F_\gamma = \{\boldsymbol{n}(\theta)/\gamma(\boldsymbol{n}(\theta)) \,|\, \theta \in S^1 = \mathbb{R}/2\pi\mathbb{Z}\}$ is a convex polygon, γ is called *crystalline energy*. When F_γ is a J-sided convex polygon, there exists a set of angles $\{\phi_i \,|\, \phi_1 < \phi_2 < \cdots < \phi_J < \phi_1 + 2\pi\}$ such that the position vectors of vertices are labeled $\boldsymbol{n}(\phi_i)/\gamma(\boldsymbol{n}(\phi_i))$ in an anticlockwise order. We denote $\boldsymbol{\nu}_i = \boldsymbol{n}(\phi_i)$ $(\forall i)$. In this case, the Wulff shape, say W_γ, is also a J-sided convex polygon with the outward normal vector of the i-th edge being $\boldsymbol{\nu}_i$: $W_\gamma = \bigcap_{i=1}^{J} \{\boldsymbol{x} \in \mathbb{R}^2 \,|\, \langle \boldsymbol{x}, \boldsymbol{\nu}_i \rangle \leq \gamma(\boldsymbol{\nu}_i)\}$. Put $\mathcal{N}_\gamma = \{\boldsymbol{\nu}_1, \boldsymbol{\nu}_2, \ldots, \boldsymbol{\nu}_J\}$.

Admissible curves. Following [4], we call $\mathcal{P}$ an *essentially admissible* curve if and only if the outward unit normal vectors $\boldsymbol{n}_i, \boldsymbol{n}_{i+1} \in \mathcal{N}$ $(\boldsymbol{n}_{N+1} = \boldsymbol{n}_1)$ satisfy $\boldsymbol{\eta}/|\boldsymbol{\eta}| \notin \mathcal{N}_\gamma$ for $\boldsymbol{\eta} = (1-\lambda)\boldsymbol{n}_i + \lambda\boldsymbol{n}_{i+1}$, $\lambda \in (0, 1)$ and $i = 1, 2, \ldots, N$. Note that if $\mathcal{P}$ is an essentially admissible curve, then $\mathcal{N} \supseteq \mathcal{N}_\gamma$ holds. Moreover, $\mathcal{P}$ is an essentially admissible convex polygon if and only if $\mathcal{N} \supseteq \mathcal{N}_\gamma$ holds. We call $\mathcal{P}$ an *admissible* curve if and only if $\mathcal{P}$ is an essentially admissible curve and $\mathcal{N} \supseteq \mathcal{N}_\gamma$ holds.

Crystalline curvature. Let $\mathcal{P}$ be an essentially admissible N-sided curve with the hight function $h = (h_1, h_2, \ldots, h_N)$. Then the total interfacial (crystalline) energy on $\mathcal{P}$ is $\mathcal{F}[h] = \sum_{i=1}^{N} \gamma(\boldsymbol{n}_i) d_i[h]$. We call negative of the first variation of $\mathcal{F}[h]$ *crystalline curvature* of $\mathcal{P}$ at $\mathcal{S}_i$ and denote it by $\Lambda_\gamma(\boldsymbol{n}_i)$:

$$\Lambda_\gamma(\boldsymbol{n}_i) = -\frac{\partial \mathcal{F}[h]}{\partial h_i} = \frac{\chi_i l_\gamma(\boldsymbol{n}_i)}{d_i[h]}, \quad i = 1, 2, \ldots, N,$$

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where χ_i takes $+1$ (resp. -1) if $\mathcal{P}$ is concave (resp. convex) around $\mathcal{S}_i$ in the direction of $\boldsymbol{n}_i$, otherwise $\chi_i = 0$, and $l_\gamma(\boldsymbol{n})$ is the lenth of the j-th edge of W_γ if $\boldsymbol{n} = \boldsymbol{\nu}_j$ for some j, otherwise $l_\gamma(\boldsymbol{n}) = 0$. Note that if $\mathcal{P}$ is an admissible and convex polygon, then $\boldsymbol{n}_i = \boldsymbol{\nu}_i$ and $\chi_i = -1$ for all $i = 1, 2, \ldots, N = J$; and moreover, if $\mathcal{P} = W_\gamma$, then the crystalline curvature is -1.

An area-preserving motion by crystalline curvature. The gradient flow of $\mathcal{F}$ along $\mathcal{P}$ which encloses a fixed area is

$$\frac{d}{dt}h_i(t) = \Lambda_\gamma(\boldsymbol{n}_i) - \overline{\Lambda}_\gamma, \quad i = 1, 2, \ldots, N, \tag{2}$$

where $\overline{\Lambda}_\gamma$ is the average of the crystalline curvature: $\overline{\Lambda}_\gamma = \dfrac{\sum_{j=1}^N \chi_j l_\gamma(\boldsymbol{n}_j)}{\sum_{k=1}^N d_k}$. Hereafter we use the notation $\dot{u} = du/dt$. In (2), $\dot{h}_i$ is the normal velocity, say v_i, of $\mathcal{S}_i$ in the direction $\boldsymbol{n}_i$. Then from (1), we have

$$\dot{d}_i = -(\cot\vartheta_i + \cot\vartheta_{i+1})v_i + v_{i-1}\operatorname{cosec}\vartheta_i + v_{i+1}\operatorname{cosec}\vartheta_{i+1}, \quad i = 1, 2, \ldots, N. \tag{3}$$

Furthermore, we have

$$\dot{\boldsymbol{p}}_i = v_i\boldsymbol{n}_i + \frac{v_{i-1} - \langle \boldsymbol{n}_{i-1}, \boldsymbol{n}_i\rangle v_i}{\langle \boldsymbol{n}_{i-1}, \boldsymbol{t}_i\rangle}\boldsymbol{t}_i, \quad i = 1, 2, \ldots, N, \tag{4}$$

from the relation $v_i = \dot{h}_i$ and

$$\boldsymbol{p}_i = h_i\boldsymbol{n}_i + \frac{h_{i-1} - \langle \boldsymbol{n}_{i-1}, \boldsymbol{n}_i\rangle h_i}{\langle \boldsymbol{n}_{i-1}, \boldsymbol{t}_i\rangle}\boldsymbol{t}_i, \quad i = 1, 2, \ldots, N.$$

Note that (2), (3) and (4) are equivalent each other.

Problem. For a given essentially admissible curve $\mathcal{P}_0$, find a family of essentially admissible curves $\{P(t)\}_{0\le t<T}$ satisfying (2) (or (3) or (4)) with $\mathcal{P}(0) = \mathcal{P}_0$. Since (3) are the system of ODEs, the maximal existence time is positive: $T > 0$.

Two basic properties. One is that the total energy $\mathcal{F}(t) = \mathcal{F}[h(t)]$ is decreasing in time: $\dot{\mathcal{F}}(t) \le 0$. The other is that the area enclosed by $\mathcal{P}(t)$, say $\mathcal{A}(t)$, is preserved: $\dot{\mathcal{A}}(t) = 0$.

Aims. The aims of this talk are to construct a numerical scheme which enjoys the above basic properties, and to investigate what might happen to $\mathcal{P}(t)$ as t tends to $T \le \infty$.

2. Numerical scheme

We discretize the system of ordinary equations (2) or (3) or (4) with the initial curve $\mathcal{P}^0 = \mathcal{P}_0$. Let $m = 0, 1, 2, \ldots$ be a step number.

Procedure A (extension of [7]) Fix parameters $\mu \in [0, 1]$ and $\lambda, \varepsilon \in (0, 1)$. For a given essentially admissible N-sided curve $\mathcal{P}^m = \bigcup_{i=1}^N [\boldsymbol{p}_i^m, \boldsymbol{p}_{i+1}^m]$, we define $\mathcal{P}^{m+1} = \bigcup_{i=1}^N [\boldsymbol{p}_i^{m+1}, \boldsymbol{p}_{i+1}^{m+1}]$ as follows:

(i) the i-th length: $d_i^m = |\boldsymbol{p}_{i+1}^m - \boldsymbol{p}_i^m|$ $(\forall i)$;

(ii) the time step: $\tau_m = \rho(d_{\min}^m)^2/\Delta$, where
$\rho = \varepsilon(1 - \mu\lambda)\min\{\lambda, 1 - \mu\lambda\}$, $\Delta = 2|\chi l_\gamma(\boldsymbol{n})|_{\max}(2/|\sin\vartheta|_{\min} + |\tan(\vartheta/2)|_{\max})$;

(iii) the i-th length d_i^{m+1}:
$(D_\tau d)_i^m = -(\cot\vartheta_i + \cot\vartheta_{i+1})v_i^{m+\mu} + v_{i-1}^{m+\mu}\operatorname{cosec}\vartheta_i + v_{i+1}^{m+\mu}\operatorname{cosec}\vartheta_{i+1}$ $(\forall i)$;

(iv) the i-th hight h_i^{m+1}: $(D_\tau h)_i^m = v_i^{m+\mu}$ $(\forall i)$;

(v) the i-th vertex: $\boldsymbol{p}_i^{m+1} = h_i^{m+1}\boldsymbol{n}_i + \dfrac{h_{i-1}^{m+1} - \langle \boldsymbol{n}_{i-1}, \boldsymbol{n}_i\rangle h_i^{m+1}}{\langle \boldsymbol{n}_{i-1}, \boldsymbol{t}_i\rangle}\boldsymbol{t}_i$ $(\forall i)$.

Here we have used the notation: $a_{\min} = \min_i a_i$, $|a|_{\min} = \min_i |a_i|$, $|a|_{\max} = \max_i |a_i|$, and $(D_\tau a)_i^m = (a_i^{m+1} - a_i^m)/\tau_m$.

Two basic properties. One is that the total energy $\mathcal{F}^m$ is decreasing in steps: $(D_\tau \mathcal{F})^m \leq 0$ for any $\mu \in [0,1]$. The other is that the area enclosed by $\mathcal{P}^m$, say $\mathcal{A}^m$, is preserved: $(D_\tau \mathcal{A})^m = 0$ if $\mu = 1/2$.

Iteration. In (iii), if $\mu \in (0,1]$, we solve the following iteration starting from $z_i^0 = d_i^m$:

$$\frac{z_i^{k+1} - z_i^0}{\tau_m} = -(\cot\vartheta_i + \cot\vartheta_{i+1})\widetilde{v}_i^{m+\mu} + \widetilde{v}_{i-1}^{m+\mu}\operatorname{cosec}\vartheta_i + \widetilde{v}_{i+1}^{m+\mu}\operatorname{cosec}\vartheta_{i+1},$$

$$\widetilde{v}_i^{m+\mu} = \frac{\chi_i l_\gamma(\boldsymbol{n}_i)}{\widetilde{d}_i^{m+\mu}} - \frac{\sum_{j=1}^N \chi_j l_\gamma(\boldsymbol{n}_j)}{\sum_{k=1}^N \widetilde{d}_i^{m+\mu}}, \quad \widetilde{d}_i^{m+\mu} = (1-\mu)z_i^0 + \mu z_i^k, \quad k = 0, 1, \ldots$$

Convergence $\lim_{k\to\infty} z_i^k = d_i^{m+1}$ and positivity $d_i^{m+1} \geq (1-\lambda)d_i^m > 0$ hold for all i ([7]).

The maximal existence time. Since the above positivity $d_i^m > 0$ holds, we can keep iterating Procedure A in finitely many steps (even if $\mathcal{P}^m$ self-intersects at a step m, we can continue). Then the maximal existence time is $t_\infty = \lim_{m\to\infty}\sum_{k=0}^m \tau_k$. Here we have two questions: one is whether t_∞ is finite or not, and the other is what might happen to $\mathcal{P}^m$ as m tends to infinity. It is known that $t_\infty = \infty$ holds if W_γ is an N-sided regular polygon and $\mathcal{P}^0$ is an admissible convex polygon ([7]).

Extension. At the maximal existence time t_∞, it is possible that at least one edge, say the i-th edge, may disappear. If $\chi_i = 0$ or $l_\gamma(\boldsymbol{n}_i) = 0$, then $\mathcal{P}^\infty$ is still essentially admissible. Hence we can continue Procedure A starting from the initial curve $\mathcal{P}^\infty$. In practice, if some edges are small enough, we eliminate them artificially as follows.

Procedure B Put a positive parameter $\delta \ll 1$. For every step m, do the followings:

(i) define $D = \min\{d_i^m \,|\, \chi_i \neq 0,\ l_\gamma(\boldsymbol{n}_i) > 0\}$ (this is well-defined);

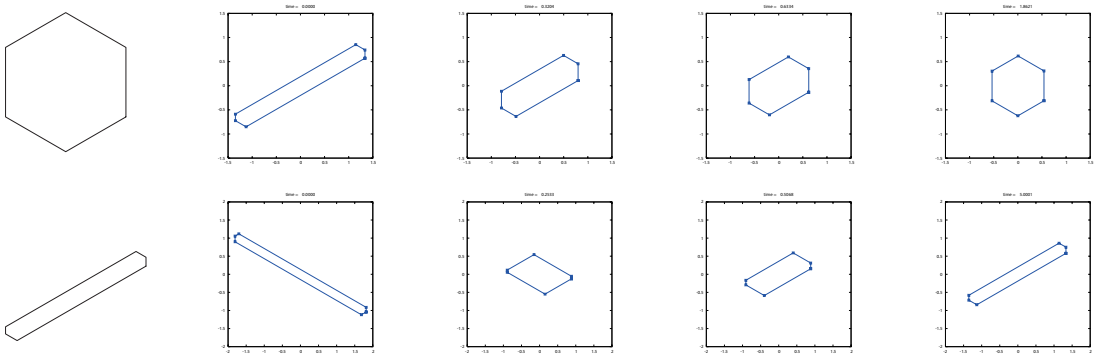
(ii) find k such that $d_k^m = \min\{d_i^m \,|\, \chi_i = 0\}$ (if it exists);
find j such that $d_j^m = \min\{d_i^m \,|\, \chi_i \neq 0,\ l_\gamma(\boldsymbol{n}_i) = 0\}$ (if it exists);

(iii) if k or j exists, check the followings:
(a) if $d_k^m/D < \delta$ and if $d_k^m \leq d_j^m$ or j does not exist, eliminate the k-th edge;
(b) if $d_j^m/D < \delta$ and if $d_j^m < d_k^m$ or k does not exist, eliminate the j-th edge;
(c) otherwise, exit from Procedure B.

3. Numerical simulations

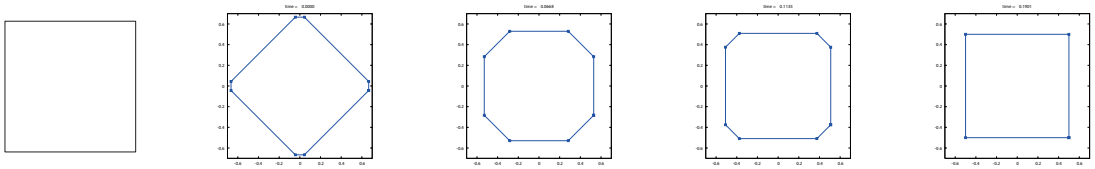
In the following five figures on each line, from left to right, they indicate W_γ, $\mathcal{P}^0$, $\mathcal{P}^{m_1}$, $\mathcal{P}^{m_2}$, $\mathcal{P}^{m_3}$ $(0 < m_1 < m_2 < m_3)$.

The case where $\mathcal{P}_0$ is convex and admissible. The solution polygon $\mathcal{P}(t)$ exists globally in time, and $\mathcal{P}(t)$ converges to W_γ as t tends to infinity. See [8] in the case $\gamma = const.$, and [9, PartI] in general. See also [2] for the smooth case. On the convergence between $\mathcal{P}(t_m)$ and $\mathcal{P}^m$, see [7].

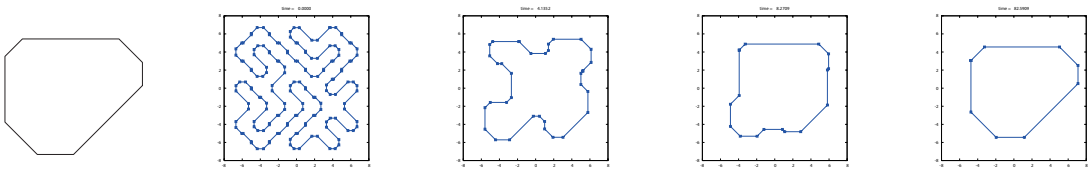


The case where $\mathcal{P}_0$ is convex and essentially admissible. By a similar proof as in [8] or [10], it can be proved that if the maximal existence time $T < \infty$ and the i-th edge disappears as t

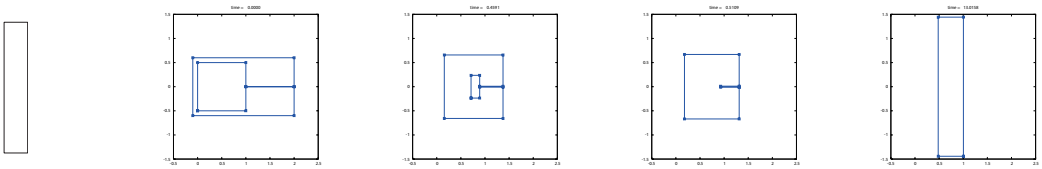
tends to T, then $l_\gamma(\boldsymbol{n}_i) = 0$. That is, the normal vector of vanishing edge does not belong to $\mathcal{N}_\gamma$, and $\inf_{0<t<T}\{d_i(t) \,|\, l_\gamma(\boldsymbol{n}_i) > 0\} > 0$ holds.



The case where $\mathcal{P}_0$ is nonconvex and admissible. The following figure indicates convexified phenomena.



In smooth case, a self-intersection is conjectured in [2], and is proved in [5]. The following figure is a numerical example of self-intersection.



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CRS: a fast algorithm based on Bi-CR for solving nonsymmetric linear systems

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Abstract. Recently, the Conjugate Residual (CR) method has been extended to nonsymmetric linear systems [8][9] and it is known that the algorithm (Bi-CR) often shows smoother convergence behavior than Bi-CG [1] in terms of the residual 2-norm. In this paper, based on product-type methods of Bi-CR, a Conjugate Residual Squared (CRS) method is proposed for solving nonsymmetric linear systems. Numerical experiments show that CRS often converges faster and generates more accurate solutions than CGS [10].

1 Introduction

We consider the solution of large and sparse nonsymmetric linear systems of the form

$$A\boldsymbol{x} = \boldsymbol{b} \quad \text{with } A \in R^{N\times N},\ \boldsymbol{x}, \boldsymbol{b} \in R^N. \tag{1.1}$$

In the last few decades Krylov subspace (KS) methods have been recognized as a class of fast solvers for the above systems and many solvers have been proposed according to the user needs; see, e.g., the recent surveys [2][3][7] and books [6][13]. Of the KS methods, the bi-conjugate gradient (Bi-CG) method [1] that can be regarded as a natural extension of the conjugate gradient (CG) method [4] plays a very important role in designing recent fast solvers such as CGS [10], Bi-CGSTAB [12], and GPBi-CG [14]. Since these successful variants of Bi-CG are obtained by the product of the corresponding matrix polynomial and the Bi-CG residual, they are often referred to as *product-type methods*.

On the other hand, recently the bi-conjugate residual (Bi-CR) method [8][9] has been proposed for solving (1.1), which is regarded as a natural extension of the conjugate residual (CR) method [11]. Since Bi-CR often shows smoother convergence behavior than Bi-CG in the residual 2-norm, Bi-CR can be expected to become an attractive basic solver for the *product-type methods*.

The purpose of this paper is to consider the *product-type methods* based on Bi-CR. In this paper, we give one of the *product-type methods* on the analogy of CGS and the resulting algorithm is referred to as conjugate residual squared (CRS).

This paper is organized as follows. In §2, we give a framework of the product type methods based on Bi-CR and derive CRS from the analogy of CGS. In §3, we report the results of some numerical experiments. Finally, we make some concluding remarks in §4.

2 A conjugate residual squared method

In this section, we give a framework of *product-type methods* based on Bi-CR and then describe the idea and the algorithm of CRS.

We define the nth residual vector of the *product-type methods* based on Bi-CR as the product of matrix polynomial of order n and the nth Bi-CR residual vector as follows:

$$\boldsymbol{r}_n := H_n(A)\boldsymbol{r}_n^{\mathrm{BiCR}} = H_n(A)R_n(A)\boldsymbol{r}_0, \tag{2.1}$$

where $R_n(A)$ is the Bi-CR residual polynomial and is explicitly written as coupled two-term recurrences with scalar λ below.

$$R_0(\lambda) \quad = \quad 1, \quad P_0(\lambda) = 1, \tag{2.2}$$

$$R_n(\lambda) = R_{n-1}(\lambda) - \alpha_{n-1}\lambda P_{n-1}(\lambda), \tag{2.3}$$

$$P_n(\lambda) = R_n(\lambda) + \beta_{n-1}P_{n-1}(\lambda), \quad n = 1, 2, \ldots \tag{2.4}$$

We can see from (2.1) that the choice of H_n is important to accelerate the speed of convergence of Bi-CR. Here, we choose H_n to be the same matrix polynomial of Bi-CR, i.e. $H_n = R_n$. This idea is closely related to the choice for CGS [10], see also [14]. Then from (2.1) and the choice $H_n = R_n$ we have

$$\boldsymbol{r}_n = H_n(A)\boldsymbol{r}_n^{\mathrm{BiCR}} = R_n(A)^2\boldsymbol{r}_0. \tag{2.5}$$

Since the above residual vector is updated by the square of Bi-CR polynomials, we name the resulting algorithm Conjugate Residual Squared (CRS). The rest of this section describes formulas for updating (2.5) and the CRS algorithm. It follows from (2.5), the recurrence relations (2.2)-(2.4), and auxiliary vectors

$$\boldsymbol{e}_n := P_n(A)R_n(A)\boldsymbol{r}_0, \quad \boldsymbol{h}_n := P_n(A)R_{n+1}(A)\boldsymbol{r}_0, \quad \boldsymbol{p}_n := P_n(A)P_n(A)\boldsymbol{r}_0$$

that we obtain recurrences for updating $\boldsymbol{r}_{n+1}$ as follows:

$$A\boldsymbol{p}_n = A\boldsymbol{e}_n + \beta_{n-1}(A\boldsymbol{h}_{n-1} + \beta_{n-1}A\boldsymbol{p}_{n-1}), \tag{2.6}$$

$$\boldsymbol{h}_n = \boldsymbol{e}_n - \alpha_n A\boldsymbol{p}_n, \tag{2.7}$$

$$\boldsymbol{r}_{n+1} = \boldsymbol{r}_n - \alpha_n A(\boldsymbol{e}_n + \boldsymbol{h}_n),$$

$$\boldsymbol{e}_{n+1} = \boldsymbol{r}_{n+1} + \beta_n \boldsymbol{h}_n. \tag{2.8}$$

The values of two parameters α_n and β_n must be equivalent to ones with Bi-CR [8]. Hence, we use the following relations:

$$\alpha_n = \frac{(\boldsymbol{r}_n^{\mathrm{BiCR}*}, A\boldsymbol{r}_n^{\mathrm{BiCR}})}{(A^T\boldsymbol{p}_n^{\mathrm{BiCR}*}, A\boldsymbol{p}_n^{\mathrm{BiCR}})} = \frac{(R_n(A^T)\boldsymbol{r}_0^*, AR_n(A)\boldsymbol{r}_0)}{(A^TP_n(A^T)\boldsymbol{r}_0^*, AP_n(A)\boldsymbol{r}_0)} = \frac{(\boldsymbol{r}_0^*, AR_n(A)R_n(A)\boldsymbol{r}_0)}{(\boldsymbol{r}_0^*, A^2P_n(A)P_n(A)\boldsymbol{r}_0)},$$

$$\beta_n = \frac{(\boldsymbol{r}_n^{\mathrm{BiCR}*}, A\boldsymbol{r}_n^{\mathrm{BiCR}})}{(\boldsymbol{r}_{n+1}^{\mathrm{BiCR}*}, A\boldsymbol{r}_{n+1}^{\mathrm{BiCR}})} = \frac{(R_n(A^T)\boldsymbol{r}_0^*, AR_n(A)\boldsymbol{r}_0)}{(R_{n+1}(A^T)\boldsymbol{r}_0^*, AR_{n+1}(A)\boldsymbol{r}_0)} = \frac{(\boldsymbol{r}_0^*, AR_n(A)R_n(A)\boldsymbol{r}_0)}{(\boldsymbol{r}_0^*, AR_{n+1}(A)R_{n+1}(A)\boldsymbol{r}_0)}.$$

Then, from the definitions of $\boldsymbol{r}_n$ and $\boldsymbol{p}_n$ we have

$$\alpha_n = \frac{(\boldsymbol{r}_0^*, A\boldsymbol{r}_n)}{(\boldsymbol{r}_0^*, A^2\boldsymbol{p}_n)}, \quad \beta_n = \frac{(\boldsymbol{r}_0^*, A\boldsymbol{r}_n)}{(\boldsymbol{r}_0^*, A\boldsymbol{r}_{n+1})}. \tag{2.9}$$

Now, we can update CRS residuals by the above recurrences. However, in terms of computational cost, it requires 4 matrix-vector multiplications per iteration. To reduce this cost, we introduce the following auxiliary recurrences:

$$A\boldsymbol{h}_n = A\boldsymbol{e}_n - \alpha_n A^2\boldsymbol{p}_n, \quad A\boldsymbol{e}_{n+1} = A\boldsymbol{r}_{n+1} + \beta_n A\boldsymbol{h}_n. \tag{2.10}$$

This leads to 2 matrix-vector multiplications per iteration. Here, we define $\boldsymbol{q}_n := A\boldsymbol{p}_n$, $\boldsymbol{d}_n := A\boldsymbol{e}_n$, and $\boldsymbol{f}_n := A\boldsymbol{h}_n$. Then, (2.6) and (2.10) are rewritten as

$$\boldsymbol{q}_n = \boldsymbol{d}_n + \beta_{n-1}(\boldsymbol{f}_{n-1} + \beta_{n-1}\boldsymbol{q}_{n-1}), \tag{2.11}$$

$$\boldsymbol{f}_n = \boldsymbol{d}_n - \alpha_n A\boldsymbol{q}_n, \tag{2.12}$$

$$\boldsymbol{d}_{n+1} = A\boldsymbol{r}_{n+1} + \beta_n \boldsymbol{f}_n. \tag{2.13}$$

Finally, the $(n+1)$th residual vector and the approximate solution are updated by

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \alpha_n(\boldsymbol{e}_n + \boldsymbol{h}_n), \quad \boldsymbol{r}_{n+1} = \boldsymbol{r}_n - \alpha_n(\boldsymbol{d}_n + \boldsymbol{f}_n). \tag{2.14}$$

From (2.7)-(2.9) and (2.11)-(2.14), we obtain the algorithm of CRS below.

Algorithm 1. Conjugate residual squared (CRS) method

$\boldsymbol{x}_0$ is an initial guess, $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$,
choose $\boldsymbol{r}_0^*$ (for example, $\boldsymbol{r}_0^* = \boldsymbol{r}_0$),
set $\boldsymbol{e}_0 = \boldsymbol{r}_0,\ \boldsymbol{d}_0 = A\boldsymbol{e}_0,\ \beta_{-1} = 0$,
for $n = 0, 1, \ldots,$ until $\|\boldsymbol{r}_n\| \le \epsilon\|\boldsymbol{b}\|$ do:

$$\boldsymbol{q}_n = \boldsymbol{d}_n + \beta_{n-1}(\boldsymbol{f}_{n-1} + \beta_{n-1}\boldsymbol{q}_{n-1}),$$
$$\alpha_n = \frac{(\boldsymbol{r}_0^*, A\boldsymbol{r}_n)}{(\boldsymbol{r}_0^*, A\boldsymbol{q}_n)},$$
$$\boldsymbol{h}_n = \boldsymbol{e}_n - \alpha_n\boldsymbol{q}_n,$$
$$\boldsymbol{f}_n = \boldsymbol{d}_n - \alpha_n A\boldsymbol{q}_n,$$
$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \alpha_n(\boldsymbol{e}_n + \boldsymbol{h}_n),$$
$$\boldsymbol{r}_{n+1} = \boldsymbol{r}_n - \alpha_n(\boldsymbol{d}_n + \boldsymbol{f}_n),$$
$$\beta_n = \frac{(\boldsymbol{r}_0^*, A\boldsymbol{r}_{n+1})}{(\boldsymbol{r}_0^*, A\boldsymbol{r}_n)},$$
$$\boldsymbol{e}_{n+1} = \boldsymbol{r}_{n+1} + \beta_n\boldsymbol{h}_n,$$
$$\boldsymbol{d}_{n+1} = A\boldsymbol{r}_{n+1} + \beta_n\boldsymbol{f}_n.$$

end

3 Numerical experiments

In this section, we report the results of numerical experiments on the problems from Matrix Market (http://math.nist.gov/MatrixMarket/). The iterative solvers used in the experiments are CGS and CRS with ILU(0) preconditioning [5], and we evaluate the two methods with respect to the number of iterations (Its), computational time (Time), and $\log_{10}$ of the true relative residual 2-norm (TRR) defined as $\log_{10}\|\boldsymbol{b} - A\boldsymbol{x}_n\|/|\boldsymbol{b}\|$. All experiments were performed on a work station with a 2.0GHz Opteron processor 846 using double precision arithmetic. Codes were written in Fortran 77 and compiled with g77 -*O*3. In all cases the iteration was started with $\boldsymbol{x}_0 = 0$ and $\boldsymbol{r}_0^* = \boldsymbol{r}_0$ in both methods, the right-hand side $\boldsymbol{b}$ was chosen as a vector with random entries from -1 to 1, and the stopping criterion was $\|\boldsymbol{r}_n\|/\|\boldsymbol{b}\| \le 10^{-12}$.

Table 1. Matrices, their sizes (N), and numerical results of CGS and CRS with ILU(0).

		Its		Time [sec]		TRR	
Matrix	N	CGS	CRS	CGS	CRS	CGS	CRS
ADD20	2395	170	151	1.55E-1	1.44E-1	-12.39	-11.99
ADD32	4960	34	34	5.65E-2	6.12E-2	-12.16	-12.04
BFW782A	782	85	85	3.25E-2	3.35E-2	-12.34	-12.25
CAVITY05	1182	123	98	1.83E-1	1.51E-1	-9.52	-11.61
CAVITY10	2597	186	181	9.26E-1	9.28E-1	-10.77	-11.57
CDDE1	961	36	37	9.02E-3	9.91E-3	-12.01	-12.38
E20R0000	4241	134	127	1.39E 0	1.34E 0	-10.04	-11.90
E30R0000	9661	257	212	6.08E 0	5.06E 0	-8.62	-10.39
FIDAP036	3079	152	160	5.69E-1	6.27E-1	-9.62	-11.89
MEMPLUS	17758	327	310	2.57E 0	3.60E 0	-9.60	-11.61
ORSIRR1	1030	47	46	1.72E-2	1.76E-2	-12.54	-12.63
ORSIRR2	886	47	47	1.47E-2	1.51E-2	-12.39	-11.99
ORSREG1	2205	53	53	3.88E-2	4.08E-2	-12.32	-12.42
PDE2961	2961	42	43	3.38E-2	3.74E-2	-12.29	-12.51
SHERMAN1	1000	41	41	9.74E-3	1.06E-2	-12.06	-12.12
SHERMAN5	3312	32	32	4.35E-2	4.65E-2	-12.46	-12.47
WATT1	1856	60	59	2.59E-2	2.75E-2	-12.18	-12.39
WATT2	1856	112	110	7.67E-2	6.14E-2	-4.52	-5.92

We evaluate the performance of CGS and CRS with ILU(0) preconditioning. The numerical results are shown in Table 1.

With respect to Its and Time, CRS only required about 80% of the iteration steps and computational time of CGS in CAVITY05 and E30R0000. There was little difference in the performance of CGS and CRS in other problems since the ILU(0) preconditioner was quite effective in improving the convergence behavior. In terms of TRR, TRRs of CRS were much better than those of CGS in CAVITY05, E30R0000, FIDAP036, and MEMPLUS. In WATT2, TRRs of the two methods were extremely less than the stopping criterion. In other problems, the two methods generated almost the same accuracy of the approximate solutions as the stopping criterion.

4 Conclusions

In this paper, on the analogy of the relationship between CGS and Bi-CG, we obtained CRS from Bi-CR. At the CJK conference we will report the residual 2-norm histories and the results of comparison of CRS with other successful solvers such as Bi-CGSTAB and GPBi-CG.

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Convergence Analysis of Nonconforming Incomplete Biquadratic Plate Element on Anisotropic Meshes*

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It is well known that the traditional finite element approximation theory relies on the regular or quasi-uniform assumption[1], i.e., there exists a constant $c > 0$, such that for all element K, $h_K/\rho_K \leq c$, or $h/\tilde{h} \leq c$, where $h = \max\limits_K h_K, \tilde{h} = \min\limits_K h_K, h_K$ and ρ_K are the diameter and the supremum of the largest inscribed circle in K respectively.

However, the domain considered may be narrow or irregular, if we seek their approximate solution with numerical calculus methods on the domain by employing the regular partition, the computing cost will be very high or can not be dealt with, it is an obvious idea to employ the anisotropic triangulation in the applications. On the other hand, solutions of some elliptic boundary problems may generate sharp boundary or interior layers, that means that the solution varies significantly in certain direction. In such case it is natural to use the meshes with small size in above direction and a large mesh size in the perpendicular direction to reflect this anisotropy in the discretization.

In the above two cases, the above assumptions are no longer valid, therefore some basic theories and techniques of the classical finite element methods are not effective. For example, when the consistency error of nonconforming element is estimated with traditional technique, $\frac{meas(F)}{meas(K)}$ is presented and might be infinite if F is a longer edge, new tricks should be explored in order to obtain convergence. On the other hand, the Sobolev interpolation theory can not be directly used on anisotropic meshes, hence the researches on the posed-well and the stability of interpolation operator are very difficult. The basic theory used to check the anisotropy of an element was given by T.Apel et al.[2,3]. But it is not convenient in application. S.C.Chen et al.[4] presented an improved one which was much easier to be used than that of [2,3]. However, the main attention of the above studies were paid to the anisotropic interpolation error analysis for the second order elliptic boundary value problems. Relatively, there are few articles considering the anisotropic nonconforming elements for the fourth order plate elements.

The objective of this paper is to discuss the convergence analysis of the incomplete biquadratic rectangular element for the fourth order plate bending problem on the anisotropic meshes. The shape function space and the degrees of freedom of the element used here are $P(K) = span\{1, x, y, x^2, xy, y^2, x^2y, xy^2\}$ or $P(K) = span\{1, x, y, x^2, xy, y^2, x^3, y^3\}$ and $\sum_K = \{v_i, \int_{\ell_i} \frac{\partial v}{\partial n} ds\}$ (i=1,2,3,4) respectively. The highlights of the work read as follows: firstly, the interpolation error estimating manner is quite different from that of [2] and [3]; secondly, by taking full advantages of the orthogonality of the quadratic part and the higher one of the element and the property of an introduced auxiliary operator, we obtain the optimal error estimate of order $O(h)$, which is similar to that of [5].

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Considering the following the biharmonic equation[1]

$$\begin{cases} \triangle^2 u = f, & in \ \ \Omega, \\ u = \frac{\partial u}{\partial n} = 0, & on \ \ \partial\Omega. \end{cases} \tag{1}$$

The corresponding variational form is to find$u \in H_0^2(\Omega)$, such that

$$a(u,v) = f(v), \ \forall \ v \in H_0^2(\Omega) \tag{2}$$

where $a(u,v) = \int_\Omega A(u,v)dxdy, \quad f(v) = \int_\Omega fvdxdy, \ A(u,v) = \Delta u \Delta v + (1-\sigma)(2u_{xy}v_{xy} - u_{xx}v_{yy} - u_{yy}v_{xx})$, $0 < \sigma < \frac{1}{2}$ is the Poisson ratio.

Let $\Omega \subset R^2$ be a domain with sides parallel to the coordinate axes, J_h be a rectangular subdivision of Ω. Let $K \in J_h$ be a rectangle, with the central point $(0,0)$, $2h_x$ and $2h_y$ ($h_x >> h_y$) the length of sides parallel to x axis and y axis respectively, $a_1(-h_x,-h_y), \ a_2(h_x,-h_y), \ a_3(h_x,h_y)$ and $a_4(-h_x,h_y)$ the four vertices, $\ell_i = \overrightarrow{a_i a_{i+1}}, \ i = 1,2,3,4, mod(4)$.

For every $v \in H^3(\Omega)$, we define the interpolation operator Π_h as follows: $\Pi_h v|_K = \Pi_K v$, and Π_K satisfies $v \in H^3(K) \to \Pi_K v \in P(K)$, such that $\Pi_K v(p_i) = v(p_i)$, $\int_{l_i} \frac{\partial \Pi_K v}{\partial n} ds = \int_{l_i} \frac{\partial v}{\partial n} ds, (i = 1,2,3,4)$. Let V_h be the associated finite element space defined as follows:

$$V_h = \{v; v|_K \in P(K), \ \forall K \in J_h, \ v_h(a) = 0, \ \int_\ell [\frac{\partial v}{\partial n}] ds = 0, \forall \ node \ a \in \partial\Omega, \ \forall \ \ell \subset \partial K\}, \tag{3}$$

Then the finite element approximation of (2) reads as: to find $u_h \in V_h$, such that

$$a_h(u_h, v_h) = f(v_h), \ \forall \ v_h \in V_h, \tag{4}$$

where $a_h(u_h,v_h) = \sum_{K \in J_h} \int_K A(u_h,v_h)dxdy, \ \forall u_h, v_h \in V_h$.

$\forall v \in H^3(K)$, let $\Pi_K v = \overline{\Pi_K v} + \Pi_K^* v$, where $\overline{\Pi_K v}$, $\Pi_K^* v$ be the quadratic term and the higher order term of $\Pi_K v$ respectively. It can be verified that the following orthogonality and the estimate hold

$$|\Pi_K v|_{2,K}^2 = |\overline{\Pi_K v}|_{2,K}^2 + |\Pi_K^* v|_{2,K}^2, \quad \|\Pi_K^* v\|_{0,K} \le Ch^2 |\Pi_K v|_{2,K}. \tag{5}$$

Now, we give the following important Lemma.

Lemma 1. $\forall \ v \in H^3(K)$, $\alpha = (\alpha_1, \alpha_2)$, $|\alpha| = 2$, there holds

$$\|D^\alpha v - D^\alpha \overline{\Pi_K v}\|_{0,K} \le \frac{h}{\pi} |v|_{3,K}. \tag{6}$$

Proof. We first prove the case $\alpha = (2,0)$. Since $\int_K D^\alpha \Pi_K^* v dxdy = 0$, we have

$$\int_K D^\alpha \overline{\Pi_K v} dxdy = \int_K D^\alpha v dxdy. \tag{7}$$

In the same way, (7) holds for the case $\alpha = (0,2)$. While for the case $\alpha = (1,1)$,

$$\begin{aligned} &\int_K D^\alpha \overline{\Pi_K v} dxdy = \int_K D^\alpha \Pi_K v dxdy = \int_K \frac{\partial^2 \Pi_K v}{\partial x \partial y} dxdy = \int_{\partial K} \frac{\partial \Pi_K v}{\partial y} \cdot n_x ds \\ &= [v(a_3) - v(a_1)] - [v(a_1) - v(a_4)] = \int_K D^\alpha v dxdy \end{aligned}$$

i.e., (7) still holds. From Poincare inequality [6], we have

$$\|D^\alpha v - D^\alpha \overline{\Pi_K v}\|_{0,K} \le \frac{h}{\pi}|D^\alpha v|_{1,K} \le \frac{h}{\pi}|v|_{3,K}. \tag{8}$$

Let u and u_h be the solutions of (2) and (4) respectively, then by Strang's second Lemma, we have

$$\|u - u_h\|_h \le C(\inf_{v_h \in V_h} \|u - v_h\|_h + \sup_{v_h \in V_h} \frac{E_h(u, v_h)}{\|v_h\|_h}), \tag{9}$$

where $E_h(u, v_h) = a_h(u, v_h) - f(v_h)$, $\|\cdot\|_h = (\sum_{K\in J_h} |\cdot|^2_{2,K})^{\frac{1}{2}}$. Here and later, C is a constant independent of $\frac{h_K}{\rho_K}$ and h.

From Lemma 1, we have the following interpolation error estimate

$$\inf_{v_h \in V_h} \|u - v_h\|_h \le \|u - \overline{\Pi_K u}\|_h \le Ch|u|_{3,\Omega}, \tag{10}$$

Introducing the operator $T:\ H^1(K) \to P = span\{1, y\}$ which is defined by

$$\int_{\ell_i} Tv\mathrm{d}s = \int_{\ell_i} v\mathrm{d}s, \quad i = 1, 3. \tag{11}$$

We can prove the following conclusion.

Theorem 1. Assume $u \in H^3(\Omega) \cap H^2_0(\Omega)$, $f \in L^2(\Omega)$, then we have

$$E_h(u, v_h) \le Ch(|u|_{3,\Omega} + h\|f\|_{0,\Omega})\|v_h\|_h, \tag{12}$$

Proof. Let $\bar{v}_h$ and v^*_h be the quadratic part and the higher order term of v_h, $P^K_0 u = \frac{1}{|K|}\int_K u dxdy$, then $\int_K v^*_{hxx} dxdy = \int_K v^*_{hxy} dxdy = \int_K v^*_{hyy} dxdy = 0$, thus

$$\sum_{K\in J_h}\int_K \Delta u \Delta v^*_h dxdy = \sum_{K\in J_h}\int_K (\Delta u - P^K_0 \Delta u)\Delta v^*_h dxdy \le C\sum_{K\in J_h} h|\Delta u|_{1,K}|v^*_h|_{2,K} \le Ch|u|_{3,\Omega}\|v_h\|_h.$$

With the similar argument, we can prove that $\sum_{K\in J_h}\int_K u_{pq} v^*_{hpq} dxdy \le Ch|u|_{3,\Omega}\|v_h\|_h$, $p, q \in \{x, y\}$, which implies

$$a_h(u, v^*_h) \le Ch|u|_{3,\Omega}\|v_h\|_h. \tag{13}$$

It is easy to check that $\bar{v}_{hyy} = (T\bar{v}_{hy})_y$, $\bar{v}_{hxx} = (T\bar{v}_{hx})_x$, $\bar{v}_{hxy} = (T\bar{v}_{hx})_y = (T\bar{v}_{hy})_x$.

Let I_h be the piecewise bilinear interpolation on Ω then we have

$$\begin{aligned}
&a_h(u, \bar{v}_h) - f(v_h) = f(I_h\bar{v}_h - \bar{v}_h) + f(\bar{v}_h - v_h) + \sum_{K\in J_h}\int_K (\Delta u)_x (I_K\bar{v}_h - \bar{v}_h)_x dxdy \\
&+ \sum_{K\in J_h}\int_K (\Delta u)_y((I_K\bar{v}_h)_y - T\bar{v}_{hy})dxdy + \sum_{K\in J_h}\sum_{i=1}^4\int_{\ell_i} \Delta u(\bar{v}_{hx}n_x + T\bar{v}_{hy}n_y)ds \\
&+(1-\sigma)\{\sum_{K\in J_h}\int_K u_{xxy}(T\bar{v}_{hy} - \bar{v}_{hy})dxdy + \sum_{K\in J_h}\int_K u_{xxy}(\bar{v}_{hx} - T\bar{v}_{hx})dxdy \\
&+ \sum_{K\in J_h}\sum_{i=1}^4\int_{\ell_i} u_{xy}\bar{v}_{hy}n_x ds - \sum_{K\in J_h}\sum_{i=1}^4\int_{\ell_i} u_{xx}T\bar{v}_{hy}n_y ds \\
&+ \sum_{K\in J_h}\sum_{i=1}^4\int_{\ell_i} u_{xy}T\bar{v}_{hx}n_y ds - \sum_{K\in J_h}\sum_{i=1}^4\int_{\ell_i} u_{yy}\bar{v}_{hx}n_x ds\} = \sum_{i=1}^4 A_i + (1-\sigma)\sum_{i=5}^{10} A_i,
\end{aligned} \tag{14}$$

Applying Schwartz inequality and the result of [2] , we have

$$A_i \le Ch^2\|f\|_{0,\Omega}\|v_h\|_h, \quad i=1,2,3,5,6. \tag{15}$$

For the term A_4, we can rewrite it as $A_4 = A_{41} + A_{42}$, where

$$A_{41} = \sum_{K\in J_h}\sum_{i=1}^{4}\int_{\ell_i}\Delta u\bar{v}_{hx}n_x ds, \quad A_{42} = \sum_{K\in J_h}\sum_{i=1}^{4}\int_{\ell_i}\Delta u T\bar{v}_{hy}n_y ds.$$

According to the result of [3], $n_y|_{F_2} = n_y|_{F_4} = 0$, and $T\bar{v}_{hy} \in span\{1, y\}$, we have

$$\begin{aligned}
A_{41} &\le C\sum_{K\in J_h}\sum_{i=1}^{4}\int_{\ell_i}\frac{|\ell_i||n_x|}{|K|}(\sum_{q\in\{x,y\}}h_q^2\|\partial_q\Delta u\|_{0,K}^2)^{\frac{1}{2}}(\sum_{q\in\{x,y\}}h_q^2\|\partial_q\bar{v}_{hx}\|_{0,K}^2)^{\frac{1}{2}} \le Ch|u|_{3,\Omega}\|v_h\|_h\\
A_{42} &\le C\sum_{K\in J_h}\sum_{i=1}^{4}\int_{\ell_i}\frac{|\ell_i||n_y|}{|K|}(\sum_{q\in\{x,y\}}h_q^2\|\partial_q\Delta u\|_{0,K}^2)^{\frac{1}{2}}(\sum_{q\in\{x,y\}}h_q^2\|\partial_q T\bar{v}_{hy}\|_{0,K}^2)^{\frac{1}{2}}\\
&\le C\sum_{K\in J_h}\frac{h_x}{h_xh_y}(\sum_{q\in\{x,y\}}h_q^2\|\partial_q\Delta u\|_{0,K}^2)^{\frac{1}{2}}h_y\|(T\bar{v}_{hy})_y\|_{0,K} \le Ch|u|_{3,\Omega}\|v_h\|_h.
\end{aligned}$$

Thus, $A_4 \le Ch|u|_{3,\Omega}\|v_h\|_h$. Similarly, we have $A_i \le Ch|u|_{3,\Omega}\|v_h\|_h, \quad i = 7,8,9,10.$

Combining (13), (14), (15) and the above estimates follows the desired result.

Theorem 2. Under the hypothesis of Theorem 1, we have

$$\|u - u_h\|_h \le Ch(|u|_{3,\Omega} + h\|f\|_{0,\Omega}). \tag{16}$$

Finally, some numerical experiments are carried out, the results of which confirm our theoretical analysis and demonstrate a good convergence behavior of the element on anisotropic meshes.

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DDDAS Approaches to Wildland Fire Modeling

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Abstract

We report on an ongoing effort to build a Dynamic Data Driven Application System (DDDAS) for short-range forecast of weather and wildfire behavior from real-time weather data, images, and sensor streams. The system changes the forecast as new data is r eceived. We encapsulate the model code and apply an out of time-order ensemble Kalman filter in time-space with a highly parallel implementation. In this talk, we discuss how we will demonstrate that our system works using a DDDAS testbed approach and data collected from an actual fire, mathematical and computational models, and how intelligent sensors provide a symbiotic relation between data collection and modeling.

1 Introduction

We describe the current state of a dynamic data driven application system (DDDAS) for simulating wildland fires (Douglas, Beezley, Coen, Deng, Li, Mandel, Mandel, Qin, and Vodacek).

DDDAS is a paradigm whereby application (or simulations) and measurements become a symbiotic feedback control system. DDDAS entails the ability to dynamically incorporate additional data into an executing application, and in reverse, the ability of an application to dynamically steer the measurement process. Such capabilities promise more accurate analysis and prediction, more precise controls, and more reliable outcomes. The ability of an application to control and guide the measurement process and determine when, where, and how it is best to gather additional data has itself the potential of enabling more effective measurement methodologies.

Furthermore, the incorporation of dynamic inputs into an executing application invokes new system modalities and helps create application software systems that can more accurately describe real world, complex systems. This enables the development of applications that intelligently adapt to evolving conditions and that infer new knowledge in ways that are not predetermined by the initialization parameters and initial static data.

The motivation for our research is the following:

- The obvious societal value of an accurate forecast compounded with the inherent challenge in modeling nonlinear, rapidly changing phenomena.
- The difficulty in obtaining remote or in situ data.
- The challenges of communicating the on site, out of sequence data of unknown quality to remote supercomputers and using it to steer simulations.

The work necessarily extends beyond data assimilation work in progress in atmospheric or ocean sciences due to the specific application challenges: the model is strongly nonlinear and irreversible, the data arrives out of sequence from disparate data sources, and error distributions cannot be considered

Components have been developed and added to the coupled atmosphere-wildfire model which

- save, modify, and restore the state of the model,
- apply ensemble data assimilation algorithms to modify ensemble member states by comparing the data with synthetic data of the same kind created from the simulation state,
- retrieve, process, and ingest data from both novel ground-based sensors and airborne platforms in the near vicinity of a fire, and
- provide computational results visualized in several ways adaptable to user needs.

DDDAS requires sensors capable of dynamically supplying data to a simulation. An ideal sensor would be sensitive, selective, and able to communicate high level spatial and chemical information to the simulation rapidly using negligible bandwidth.

Data that come into the data center must go through a process consisting of up to six steps.

1. *Retrieval*: Get the data from sensors. This may mean receiving data directly from a sensor or indirectly through another computer or storage device (e.g., a disk drive).
2. *Extraction*: The data from some sensors may be quite messy in raw form, thus the relevant data may have to be extracted from the transmitted information.
3. *Conversion*: The units of the data may not be appropriate for our application.
4. *Quality control*: Bad data should be removed or repaired if possible. Missing data (e.g., in a composite satellite image) must be repaired.
5. *Store*: The data must be archived to the right medium (or media). This might mean a disk, tape, or computer memory, or no storage device at all (or only briefly) if data is not being archived permanently or only temporarily.
6. *Notification*: If a simulation is using the data as it comes into the data center, the application needs to be informed of the existence of new data.

2 Wildland Fire Model

The original modeling system is composed of two parts: a numerical weather prediction model and a fire behavior model that models the growth of a wildfire in response to weather, fuel conditions, and terrain (Clark, Coen, and Latham 2004, Coen 2005). These models are two way coupled so that heat and water vapor fluxes from the fire are released into the atmosphere, affecting the winds in particular, while the fire affected winds feed back upon the fire propagation. This wildfire simulation model can thus represent the complex interactions between a fire and the atmosphere.

The meteorological model is a three-dimensional non-hydrostatic numerical model based on the Navier-Stokes equations of motion, a thermodynamic equation, and conservation of mass equations using the anelastic approximation. Vertically-stretched terrain-following coordinates allow the user to simulate in detail the airflow over complex terrain. Gridded natioinal weather forecasts are used to initialize the domain and update lateral boundary conditions. Two-way interactive nested grids capture the outer forcing domain scale of the synoptic-scale environment while allowing the user to telescope down to tens of meters near the fireline through horizontal and vertical grid refinement. Weather processes such as the production of cloud droplets, rain, and ice are parameterized using standard treatments.

In the original model, local fire spread rates depend on the modeled wind components, fuel properties, and terrain slope through an application of the semi-empirical Rothermel fire spread formula (Rothermel 1972). We are replacing the Rothermel model with a simple physics and PDE based model (Mandel, Chen, Franca, Johns, Puhalskii, Coen, Douglas, Kremens, Vodacek, and Zhao 2004). This PDE model uses the reaction-convection-diffusion equation for the tempera-

ture T and fuel supply S,

$$c\frac{\partial T}{\partial t} = -\nabla d \nabla T - av \cdot \nabla T + e\frac{\partial S_k}{\partial t} - b\left(T - T_a\right), \quad (1)$$

$$\frac{\partial S}{\partial t} = -f(T)S. \quad (2)$$

(1) is the balance of heat. The term $-\nabla d \nabla T$ models the heat diffusion, $-av \cdot \nabla T$ is the convection by wind with speed v, $e\frac{\partial S_k}{\partial t}$ is the heat generated by burning the fuel, and $-b\left(T - T_a\right)$ is the heat lost to the ambient environment with temperature T_a. (2) is the balance of fuel. This simple model is capable of producing a reasonable fire behavior with an advancing fire front. A more advanced version of this model is under development, which will include several species of fuel, radiative heat transfer between fuel species, and evaporation of moisture. It is anticipated that this model will replace the empirical fire model and it will be coupled to the atmospheric model. For related physics based fire models in the literature, see, e.g., (Linn, Reisner, Colman, and Winterkamp 2002, Serón, Gutiérrez, Magallón, Ferragut, and Asensio 2005).

Forecasting with the coupled atmosphere fire model is achieved using the Ensemble Kalman Filter (EnKF). Ensemble filters work by advancing in time a collection of simulations started from randomly perturbed initial conditions. When the data is injected, the ensemble (called *forecast*) is updated to get a new ensemble (called *analysis*) to achieve a least squares fit using two conditions: the change in the ensemble members should be minimized, and the data d should fit the ensemble members state u,

$$h(u) \approx d, \quad (3)$$

where h is called the *observation function*. The weights in the least squares are obtained from the covariances of the ensemble and of the data error. For comprehensive surveys of EnKF techniques, see (Evensen 2003, Evensen 2004, Tippett, Anderson, Bishop, Hamill, and Whitaker 2003). In general, *EnKF works by forming the analysis ensemble as linear combinations of the forecast ensemble.*

We are using filters based on the EnKF with data perturbation (Burgers, van Leeuwen, and Evensen 1998). But, even with the simple wildfire model (1)-(2), the data assimilation produces an ensemble with nonphysical solutions causing the simulations to break down numerically. Therefore, we have proposed a regularization by adding a term involving the change in the spatial gradient of ensemble members to the least squares (Johns and Mandel rint). Existing ensemble filter formulas assume that the observation function is linear, $h(u) = Hu$, and then compute with the observation matrix H. To simplify the software, we have derived a mathematically equivalent ensemble filter that only needs to evaluate $h(u)$ for each ensemble member.

For the issue of assimilating of out-of-order data we will use system states that combine states at several times (Mandel, Chen, Franca, Johns, Puhalskii, Coen, Douglas, Kremens, Vodacek, and Zhao 2004). The parallel computing framework we have developed was designed with this in mind.

Data comes from fixed ground sensors that measure temperature, radiation, and local weather conditions (Kremens, Faulring, Gallagher, Seema, and Vodacek 2003). These systems will survive burn-over by low intensity fires and are intended to supplement other sources of weather data derived from permanent and portable automated weather stations. The temperature and radiation measurements provide the direct indication of the fire front passage and the radiation measurement can also be used to determine the intensity of the fire.

Data also come from images taken by sensors on either satellites or airplanes. The primary source of image data is the Wildfire Airborne Sensor Project (WASP) (Li, Vodacek, Kremens, Ononye, and Tang 2005). This three wavelength digital infrared camera system is carried on an airplane that is flown over the fire area. Camera calibration, an inertial measurement unit, GPS, and digital elevation data are used in a processing system to convert raw images to a map product with a latitude and longitude associated with each pixel. The three wavelength infrared images can then be processed using a variety of algorithm approaches (Li, Vodacek, Kremens, Ononye, and Tang 2005, Dozier 1981) to extract which pixels contain a signal from fire and to determine the energy radiated by the fire (Wooster, Zhukov, and Oertel 2003, Smith, Wooster, Drake, Perry, Dipotso, Falkowski, and Hudak 2005).

The data are related to the model by the observation equation (3). The observation function h maps the system state u to *synthetic data*, which are the values the data would be in the absence of modeling and measurement errors. Knowledge of the observation function, the data, and an estimate of the data error covariance is enough to find the correct linear combinations of ensemble members in the ensemble filter. The data assimilation code also requires an approximate inverse g of the observation function. For a system state u and data d, $g\left(h(u) - d\right)$ is the direction in which the system state can change to decrease a norm of the data residual $h\left(u\right) - d$. For an observation function that is simply the value of a variable in the system state, the natural choice of approximate inverse can be just the corresponding term of the data residual, embedded in a zero vector.

Building the observation function and its approximate inverse requires conversion of physical units be-

tween the model and data and conversion and interpolation of physical coordinates. In addition, synthetic data at instants of time between the simulation time of ensemble members need to be interpolated to the data time. The data injection itself is done by updating the ensemble to minimize a weighted sum of the data residual and the change in the ensemble.

The data items enter in a pool maintained by the data acquisition module. The assimilation code can query the data acquisition module to determine if there are any new data items available, request their quantitative and numerical properties, and delete them from the pool after they are no longer needed.

3 Conclusions

The wildland fire DDDAS provides a rich, multidisciplinary environment where researchers in mathematics, atmospheric sciences, imaging sciences, and sensor design. There are open questions in each of these fields related to this one DDDAS project that need to be addressed in order to provide a comprehensice and solid scientific basis for the computations.

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Analysis of conforming and nonconforming finite element methods in wave propagation

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In the first part of this presentation we will review several nonconforming elements in two and three dimensions. In 1973 the linear nonconforming finite elements for triangles or tetrahedrons and a cubic nonconforming element for triangles by Crouzeix and Raviart citecr73. Corresponding quadrilateral elements have been proposed [23] by Han [10], and Rannacher and Turek, and later the DSSY nonconforming element introduced by Douglas *et al.* [6]. Such nonconforming elements have been proved very effectively applicable to fluid mechanics [25] and elasticity [3, 16, 13, 14].

The P_1-nonconforming quadrilateral and hexahedral finite element introduced [22, 8]. A quadratic nonconforming element on rectangle has been proposed [18]. Notice that our element is different from the incomplete biquadratic element [24]. The incomplete biquadratic element has degrees of freedom similar to those of Morley's element [20], which consist of values at vertices and normal derivative values at midpoints of edges, while our element has those similar to the element of Fortin and Soulie [7, 17], which consist of values at two Gauss points of each edge. Instead of using standard conforming finite elements in domain decomposition methods, the use of nonconforming finite elements has shown to have certain advantages as the amount of interchange of informations between neighboring processors is reduced compared to using conforming elements. Also, an actual radius of convergence of domain decomposition iteration can be shown if nonconforming elements are used instead of conforming elements [6, 15, 9]. Several aspects of comparative analyses of the above three elements in two or three dimensional problems will be discussed. The construction of basis functions and their dimensions will be discussed depending on the choice between Dirichlet and Neumann type boundary conditions.

In the second part of the presentation we analyze the numerical dispersion relation of some conforming and nonconforming quadrilateral finite elements. The finite difference method has been widely used to solve wave propagation problems due to its simplicity in implementation [2, 19] However, if the underlying domain geometries are irregular or the wave speed is highly discontinuous, the finite element method with suitable adaptive mesh generation will give more precise numerical solutions at reasonable computational costs, compared to the finite difference method. Three-dimensional problems usually require huge memories and long computation time, and thus parallelization techniques, such as domain decomposition methods, are usually adopted.

The first finite element error analysis for Helmholtz problem was given by Douglas-Santos-Sheen-Bennethum [5] for one dimension. Among other contributions made by this paper, obtained were important error bounds that depend on both the spatial mesh size h and frequency ω. Based

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on this work, Babuska and Ihrenburg [12], and their colleagues, raised an important issue, what is called a "pollution effect", and have studied extensively to resolve it. The discrete solutions using the standard Galerkin finite element method results in inaccurate solutions if the mesh size is not sufficiently small compared to the size of wave number [1, 12, 11, 21, 5, 4], and numerical dispersion seems to be a major source for the pollution effect. Therefore, unless the size of wave number k is sufficiently small, some kind of specific finite element techniques, such as hp methods, need to be employed.

We will then examine the dispersion effects in solving Helmholtz problems by the finite element method using quadrilateral or rectangular elements of lowest order. Specifically the following three conforming and nonconforming element methods will be analyzed: (1) the standard Q_1 conforming element (abbreviated as the "Q_1 element"); (2) the DSSY nonconforming element introduced by Douglas *et al.* [6] (abbreviated as the "DSSY NC" element, or the "DSSY" element) which is a modified rotated Q_1 element of Rannacher and Turek [23]; and (3) the P_1-nonconforming quadrilateral(hexahedron) element [22] (abbreviated as the " P_1 NC element"). Santos *et al.* [27] and Zyserman *et al.* [26] gave detailed dispersion analyses for solving the Helmholtz equation, and elastic and viscoelastic equations comparing between the Q_1 conforming and the DSSY NC finite element methods. It is shown [1, 27, 26] that the L^2 error behavior of the DSSY NC element behaves better in reducing numerical dispersion than that of Q_1 element based on the same size of grids. However, it has been questionable if the DSSY NC element is actually cheaper than the Q_1 conforming element to achieve desired accuracy. One of the purposes of the our paper is to investigate in the actual costs of computation to reduce errors up to certain tolerance instead of estimating errors based on the size of meshes.

Presenting our numerical experiments, we will conclude that all the three elements selected are affected by pollution effects; however, we analyze the number of elements and the degrees of freedom necessary to guarantee the L^2 and broken H^1 errors are smaller than given tolerance ϵ. Our results imply that the P_1 NC quadrilateral elements require the least degrees of freedom among the three elements.

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Moving Mesh Methods for Singular Problems Using Perturbed Harmonic Mappings

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In this talk, we will extend Dvinsky's method to provide an efficient and practical moving mesh algorithm for solving partial differential equations.

The key idea is to construct the harmonic map between the physical space and a parameter space by an iteration procedure. Each iteration step is to move the mesh closer to the harmonic map. Thisthe map harmonic even after long time of numerical integration.

We will also discuss a recent work in developing moving mesh strategies for solving problems defined on a sphere. To construct mappings between the physical domain and the logical domain, it has been demonstrated that harmonic mapping approaches are useful for a general class of solution domains. However, it is known that the curvature of the sphere is positive, which makes the harmonic mapping on a sphere not unique. To fix the uniqueness issue, we follow Sacks and Uhlenbeck [Ann. Math., 113, 1-24 (1981)] to use a perturbed harmonic mapping in mesh generation. A detailed moving mesh strategy including mesh redistribution and solution updating on a sphere will be presented.

*This work is joint with Y. Di, R. Li and P.-W. Zhang of Peking University.

Numerical methods for wave propagation problem applied to voice generation simulation

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In this talk, we review some numerical methods for wave propagation phenomena in unbounded region and apply the methods to voice generation problem of human beings.

The basic mathematical model is the wave equation for the sound propagation in the air with the sound source at the vocal cord position. The frequency response function is the key object to simulate the voice generation process. The individual vowel is characterized by its formants that are the peaks of the frequency response function defined as the mapping from the frequency domain of the time harmonic source to the intensity of the sound pressure at a fixed observation point outside the vocal tract. Changing the shape of the vocal tract, we can produce different vowels in respective languages. In Japanese for example, there are five different vowels at the present time, and Korean has more than ten. We perform several numerical computation to compare the difference and the similarity between these two languages.

For the background of the voice generation or human speech phenomena, refer among others the books by Kent-Read[3], Childers[1] and Furui[2]. Our recent results for the voice generation problem can be seen in [4] and [5], and see [6] for the numerical method of the wave propagation in unbounded region.

For the numerical simulation of voice generation, the basic mathematical model is the Helmholtz equation. We change the frequency in the equation and calculate the frequency response function as the amplification factor of the pressure at some observation point for the given unit volume velocity of sound at the vocal cord position where the sound originates. Typical numerical example of the frequency response function computed by the finite element methods for two-dimensional cases is shown in Fig. 1 for the vowel $/a/$. We used the usual piecewise linear continuous basis functions for discretization.

In the numerical simulation of voice generation process of human beings, to investigate the relationship between the vocal tract shape and the formant curve or the frequency response function has a primal importance. For this purpose, it is very useful to investigate the complex eigenvalue problem related the Laplace operator with radiation boundary condition and the variational formula for the complex eigenvalues with respect to the deformation of vocal tract shape.

In one-dimensional case, let z and $u = u(x\,; z, A)$ be the complex eigenvalue and the eigenfunction satisfying the homogeneous Webster's horn equation for an area function $A(x)$, the variational formula is given as follows with respect

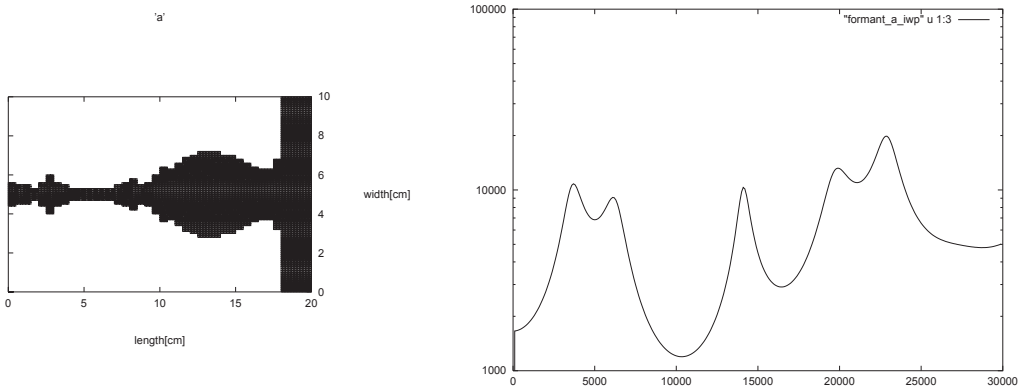

Figure 1: Two-dimensional numerical simulation of vowels /a/

to the variation $(\delta A)(x)$ of the cross section area $A(x)$ of the vocal tract:

$$\delta z = \frac{\displaystyle\int_0^L (\delta A)(x)\Big(\Big(\frac{du(x)}{dx}\Big)^2 - z^2 u(x)^2\Big)\,dx - iz(\delta A)(L)u(L)^2}{\displaystyle 2z\int_0^L A(x)u(x)^2\,dx + iA(L)u(L)^2}. \tag{1}$$

There is also the two dimensional extension of this formula. We will show some applications of this formula to design the vocal tract shape for various vowels.

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Semi-Implicit Schemes with Multilevel Wavelet-like Incremental Unknowns for a Reaction-Diffusion Equation*)

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Abstract

Incremental unknowns have been developed as a means to approximate inertial manifolds when finite differences are used. They play evidently an important role in the study of the long time behavior of the solutions of partial differential equations and in fact they produce a new and different efficient concept in finite differences which are fundamental and very useful in the field of numerical solution of partial differential equations (see e.g. [5,9,11]).

Much effort about incremental unknowns methods has been devoted in the past to the approximation of the linear elliptic equations and also some dissipative evolution equations, among them are the two-dimensional Navier-Stokes equations, the Kuramoto-Sivashinsky equations and the Burger's equations. (See also [2,6,7,12] and the references therein.)

Wavelet-like incremental unknowns (WIU) deserve special stress because they enjoy the L^2 orthogonality property between different levels of unknowns. This makes multilevel wavelet-like incremental unknowns particularly appropriate for the approximation of evolution equation (see e.g. [3,4]).

The purpose of this paper is to establish multilevel wavelet-like incremental unknowns methods for some reaction diffusion equation, especially for an equation with a polynomial growth nonlinearity of arbitrary order.

In general case, we denote by Ω an open bounded set of R^n with boundary $\Gamma = \partial\Omega$. Consider the following initial-boundary value problem involving a scalar function $u = u(x, y)$; u satisfies

$$\begin{cases} \dfrac{\partial u}{\partial t} - \nu\Delta u + g(x,u) = 0, & in \quad \Omega, \\ u(x,0) = u_0(x), & in \quad \Omega. \end{cases} \tag{1}$$

together with one of the following boundary conditions.

(i) Dirichlet type boundary condition

$$u|_\Gamma = 0 . \tag{2}$$

(ii) Neumann type boundary condition

$$\left.\frac{\partial u}{\partial \nu}\right|_\Gamma = 0 . \tag{3}$$

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2. Project partially supported by Gansu Natural Science Foundation (Grant No. 3ZS041-A25-011) and ME Foundation for University Key Teacher (Grant No. GG-110-73001-1014)

(iii)Periodicity type boundary condition

$$\Omega = (0, L)^n, \quad u \text{ is } \Omega\text{-periodic.} \tag{4}$$

Here, the function $g : \Omega \times R \to R$ is measurable in x and of class C^1 in s satisfying

$$\begin{cases} \textit{There exists } q > 2 \textit{ and } \gamma_i > 0 \textit{ such that} \\ \gamma_1 |s|^q - \gamma_0 \le g(x,s)s \le \gamma_2 |s|^q + \gamma_3, \quad \forall s \in R^+, \ a.\ e.\ x \in \Omega \end{cases} \tag{5}$$

and

$$\begin{cases} \textit{There exists } \gamma_4 > 0 \textit{ such that} \\ g'_s(x,s) \ge -\gamma_4, \quad \forall s \in R^+, \ a.\ e.\ x \in \Omega \end{cases} \tag{6}$$

One of the examples of our equation is the so-called Chafee-Infante equation (see e.g. [1,8])

$$\frac{\partial u}{\partial t} - \Delta u + \alpha u^3 - \beta u = 0, \qquad (\alpha, \beta > 0) \tag{7}$$

Another example we give is a certain reaction diffusion equation (see [4,8,10])

$$\frac{\partial u}{\partial t} - \nu \Delta u + g(u) = 0. \tag{8}$$

where $g(s) = \sum_{j=0}^{2p-1} b_j s^j, \quad b_{2j-1} > 0.$

For the sake of simplicity, we shall consider mainly the one dimensional case and focus particularly on the equation (8) with initial-boundary conditions. First of all, we recall the definition of the wavelet-like incremental unknowns and the exploration of the multilevel space discretization of the above problem. The equation, e.g., (8) will be expressed in terms of decomposed spaces by

$$2^d \frac{\partial \overline{U}_0}{\partial t} + \nu S^T A_d S \overline{U}_0 + S^T g(S\overline{U}_0) = 0. \tag{9}$$

Then we establish two types of semi-implicit schemes which read

Scheme I

$$\frac{2^d}{\tau} \begin{pmatrix} Y_0^{n+1} - Y_0^n \\ Z^{n+1} - Z^n \end{pmatrix} + \nu S^T A_d S \begin{pmatrix} Y_0^{n+1} \\ Z^n \end{pmatrix} + 2^d \begin{pmatrix} g(Y_0^n) \\ 0 \end{pmatrix} = 0. \tag{10}$$

Scheme II

$$\frac{2^d}{\tau} \begin{pmatrix} Y_0^{n+1} - Y_0^n \\ Z^{n+1} - Z^n \end{pmatrix} + \nu S^T A_d S \begin{pmatrix} Y_0^n \\ Z^{n+1} \end{pmatrix} + 2^d \begin{pmatrix} g(Y_0^n) \\ 0 \end{pmatrix} = 0. \tag{11}$$

They are typically of nonlinear Galerkin type.

Based on two discrete function spaces (composed of step functions)

$$Y_d = span\{\psi_{2h_d, M} \mid M = 2ih_d, \ i = 1, 2, \cdots, 2^{d-1} N\},$$

$$Z_d = span\{\chi_{2h_d,M} \mid M = (2i-1)h_d,\ i = 1,2,\cdots,2^{d-1}N\},$$

we are able to obtain the equivalent variational formulations of our finite differences in wavelet-like incremental unknowns. Afterwards, we analyze the stability of the schemes through the variational formulations and prove the stability theorems. The limitation of time mesh $\tau = \Delta t$ is obviously better than that obtained with standard one-level spatial discretization. The stability conditions are improved when compared with explicit schemes in WIU. Stability conditions both for Scheme II and classic implicit scheme are comparable if d is sufficiently large. Finally, we show some numerical results and give probably further expectation.

Keywords: Wavelet-like incremental unknowns, reaction diffusion equation, nonlinear Galerkin method, semi-implicit schemes

AMS Subject Classification: 65M60, 65M06, 35K60

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Mathematical Modeling for Moisture Transport in Fibrous Materials and Applications.

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Mass and heat transfer in fibrous porous media can be found in numerous industrial and engineering applications such as textile, paper and pulp, building materials and more recently in the electrodes of proton exchange membrane fuel cells. In these applications, modeling becomes increasing important since it provides an efficient and cost effective way for evaluating new designs or testing new materials.

Theoretical modeling of coupled heat and moisture transfer with phase change in fibrous insulation started with Henry's work in the 1930s. However, little progress was made until the 1980s and 1990s when several researchers investigated the problems related textile and insulation materials using analytical and numerical methods. Due to recent interests in PEM fuel cells, multi-component modeling and mathematical analysis haven also been carried out for reactant and moisture transport in hydrophobic fibrous media when it is relevant. In the context of fibrous clothing assemblies, Fan et al. introduced dynamic moisture absorption and radiation heat transfer into the existing models and consequently they achieved better agreement with experimental measurements.

In this talk, we present our recent work on moisture transport model in fibrous clothing assemblies in a one dimensional setting. We formulate this problem as multi-phase flows in fibrous porous media with phase change. The model is based on a previous study with significant modification to take into account the air resistance to moisture transport as well as the capillary effect on liquid water motion. By the conservation of mass for vapor, air, and liquid as well as conservation of energy for the mixture of gas, liquid and solid matrix, the model is described by

$$
\begin{aligned}
&\frac{\partial}{\partial t}(\epsilon C_v) + \frac{\partial}{\partial x}(u_g \epsilon C_v) = \frac{\partial}{\partial x}\left[\frac{D_g \epsilon}{\tau_c} C \frac{\partial}{\partial x}\left(\frac{C_v}{C}\right)\right] - \Gamma, \\
&\frac{\partial}{\partial t}(\epsilon C_a) + \frac{\partial}{\partial x}(u_g \epsilon C_a) = \frac{\partial}{\partial x}\left[\frac{D_g \epsilon}{\tau_c} C \frac{\partial}{\partial x}\left(\frac{C_a}{C}\right)\right], \\
&\frac{\partial}{\partial t}(C_{vt} T) + \frac{\partial}{\partial x}\left(u_g \epsilon C_{vg} T\right) = \frac{\partial}{\partial x}\left(\kappa \frac{\partial T}{\partial x}\right) + \lambda M \Gamma, \\
&\frac{\partial}{\partial t}\left[\rho(1-\epsilon')\widetilde{W}\right] + \frac{\partial(u_w \rho_w)}{\partial x} = \frac{\partial}{\partial x}\left[\rho(1-\epsilon') D_l \frac{\partial \widetilde{W}}{\partial x}\right] + M \Gamma_{ce}\,.
\end{aligned}
$$

Here the generalized Fick's law has been used for the binary multi-component gas mixture (vapor and air). C_v, C_a and $C = C_v + C_a$ are the water vapor, air and total (molar) concentrations, $\widetilde{W}$ is the liquid water content (%) on the fibre surface and u_g is the molar averaged mixture velocity. D_g is the molecular diffusion coefficient for the air and water vapor. C_{vt} and C_{vg} are the volumetric heat capacities for the mixture (gas and fibre) and vapor, respectively. κ is the heat conductivity for the gas-fibre mixture. λ is the latent heat of phase change (evaporation, condensation and freezing). Γ is the (molar) rate of phase change per unit volume and M is the molecular weight of water. τ_c is the tortuosity of the porous medium.

An efficient semi-implicit numerical scheme is proposed for solving the gas (vapor and air) and energy equations while the water equations are solved separately. Our numerical solution agrees well with the quasi-steady approximate solution. Qualitative comparison between the numerical results and the experimental measurements are also given.

Conformal Mappings to Exterior Jordan Domains and their Finite Element Approximation

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1 The problem and main idea

Let $B := \{(x, y) \in \mathbb{R}^2 | x^2 + y^2 < 1\}$ be the unit disk. Let also $\Gamma : \partial B \to \mathbb{R}^2$ be a closed Jordan curve, and D, Ω be the exterior and interior domains of Γ, respectively. By the Riemann mapping theorem, there exist conformal mappings

$$\begin{aligned}
&\varphi : B \to D, \quad \tilde{\varphi} : B \to \Omega, : \text{ conformal,} \\
&\varphi : \overline{B} - \{0\} \to \overline{D}, \quad \tilde{\varphi} : \overline{B} \to \overline{D} : \text{ homeomorphism,} \\
&\varphi(0) = \infty.
\end{aligned}$$

In this lecture, we discuss finite element approximation of the conformal mapping φ.

In [1], [2], [3], [4], we considered finite element approximation of $\tilde{\varphi} : B \to \Omega$ based on the following Dirichlet principle: Let

$$X_\Gamma := \left\{\psi \in C(\overline{B}; \mathbb{R}^2) \cap H^1(B; \mathbb{R}^2)\right\} \;\Big|\; \psi(\partial B) = \Gamma, \psi|_{\partial B} : \text{monotone}\Big\}.$$

We then have

$$\mathrm{Area}(\Omega) = \mathcal{D}_B(\tilde{\varphi}) = \min_{\psi \in X_\Gamma} \mathcal{D}_B(\psi),$$

where $\mathcal{D}_B$ is the Dirichlet integral defined by

$$\mathcal{D}_B(\psi) := \frac{1}{2} \int_B |\nabla \psi|^2 \mathrm{d}x.$$

Now, Let $\{\mathcal{T}_h\}$ be a family of regular and quasi-uniform triangulations of B and $S_h \subset H^1(B)$ be the finite element space of piecewise linear functions on $\mathcal{T}_h$. Using the Dirichlet principle, we may define the **piecewise linear finite element conformal mapping** $\tilde{\varphi}_h$ by a standard way of finite element method. Moreover, we have shown some convergence results on FE conformal mappings.

For the conformal mappings to the exterior Jordan domain D, however, we have $\mathcal{D}_B(\varphi) = \mathrm{Area}(D) = \infty$ and the above method may not be applied directly.

The main idea of this lecture is based on the fact the stereographic map (projection) $\pi : \mathbb{C} \to \mathbb{C}^*$ is conformal, where $\mathbb{C}^* := \mathbb{C} \cup \{\infty\}$, $\mathbb{C}^* \cong S^2$ is the Riemann sphere. Therefore, letting $\widetilde{D} := \pi(D) \subset \mathbb{C}^*$, we construct a conformal mapping $\phi : B \to \widetilde{D}$, $\phi(0) = \infty$, since for this ϕ, we have the Dirichlet principle similar to the above which can be used to define finite element approximation. Then, $\varphi := \phi \circ \pi^{-1}$ should be the desired conformal mapping to the exterior Jordan domain. Detailed definitions and numerical examples will be given in the lecture.

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A conservative Galerkin scheme for the KdV equation

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1 Introduction

In this talk, a new Galerkin scheme for the Korteweg-de Vries equation (KdV):

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1}{2}u^2 + \frac{\partial^2 u}{\partial x^2}\right) \qquad (x \in \mathbf{R},\ t > 0), \tag{1}$$

under the periodic boundary condition of period L, is presented. The scheme is conservative in that it has the discrete analogues of the "energy" conservation property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L \left\{\frac{1}{6}u^3 - \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2\right\}\mathrm{d}x = 0, \tag{2}$$

and the "mass" conservation property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L u\,\mathrm{d}x = 0. \tag{3}$$

The scheme is derived using the Galerkin version of the discrete variational derivative method [1, 2], which was recently proposed in [3]. In this abstract, the main results are summarized. The derivation of the scheme and numerical examples are given in the presentation.

2 The scheme and its conservativity

The scheme is shown below. Given a mesh partition on $0 \le x \le L$, let the trial space S_{d} and the test space W_{d} be the $L-$periodic piecewise linear function space over the mesh. Let also $G(u, u_x) = u^3/6 - u_x^2/2$, and $(f, g) = \int_0^L fg\,\mathrm{d}x$.

Scheme 1 (Conservative scheme for the KdV) *Let $u^{(0)}$ be given in the trial space S_{d}. Find $u^{(m+1)} \in S_{\mathrm{d}}$ and $p^{(m+\frac{1}{2})} \in S_{\mathrm{d}}$ $(m = 0, 1, \ldots)$ such that, for any $v_1,\ v_2 \in W_{\mathrm{d}}$,*

$$\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v_1\right) = \left((p^{(m+\frac{1}{2})})_x, v_1\right), \tag{4}$$

$$(p^{(m+\frac{1}{2})}, v_2) = \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}, v_2\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, (v_2)_x\right), \tag{5}$$

where

$$\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})}=\frac{(u^{(m+1)})^2+u^{(m+1)}u^{(m)}+(u^{(m)})^2}{3},\quad \frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}=\frac{u_x^{(m+1)}+u_x^{(m)}}{2}, \tag{6}$$

are discrete partial derivatives corresponding to $\partial G/\partial u$, $\partial G/\partial u_x$ *respectively.*

The conservativity of the scheme can be established as follows.

Theorem 1 (Conservativity of Scheme 1) *For* $m=0,1,2,\ldots$,

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)})-G(u^{(m)})\right)\mathrm{d}x=0,\quad \text{and}\quad \frac{1}{\Delta t}\int_0^L \left(u^{(m+1)}-u^{(m)}\right)\mathrm{d}x=0.$$

(Proof) For the first claim,

$$\begin{aligned}
&\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)})-G(u^{(m)})\right)\mathrm{d}x\\
&=\left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})},\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)+\left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})},\frac{u_x^{(m+1)}-u_x^{(m)}}{\Delta t}\right)\\
&=\left(p^{(m+\frac{1}{2})},\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)=\left(p_x^{(m+\frac{1}{2})},p^{(m+\frac{1}{2})}\right)=\frac{1}{2}\left[\left(p^{(m+\frac{1}{2})}\right)^2\right]_0^L=0.
\end{aligned} \tag{7}$$

The first equality can be checked by substituting (6) into the right hand side. The second is from (5) with $v_2=(u^{(m+1)}-u^{(m)})/\Delta t$, and the third is from (4) with $v_1=p^{(m+\frac{1}{2})}$; these substitutions are allowed since $S_{\mathrm{d}}=W_{\mathrm{d}}$. Similarly, the second claim is obtained by

$$\frac{1}{\Delta t}\int_0^L \left(u^{(m+1)}-u^{(m)}\right)\mathrm{d}x=\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t},1\right)=\left(p_x^{(m+\frac{1}{2})},1\right)=\left[p^{(m+\frac{1}{2})}\right]_0^L=0. \tag{8}$$

The second equality is from (4) with $v_1=1$. □

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The cell boundary element methods

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Abstract

We consider the model second-order elliptic problem:

$$\begin{aligned} -\nabla \cdot K\nabla u &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{1}$$

where Ω is a bounded polygonal domain in $\mathbb{R}^2$. Assume that Ω is composed of disjoint polygonal subdomains $\Omega_1, \cdots, \Omega_J$ and that K is a function such that $0 < K_* \leq K(x) \leq K^* < \infty$ and $K(x) = K_j$ in Ω_j for each j.

The localized problem becomes

$$\begin{aligned} -K_T \Delta u &= f \quad \text{in } T, \\ \left[K\frac{\partial u}{\partial \nu}\right] :\equiv K_T\frac{\partial u}{\partial \nu} + K_{T'}\frac{\partial u'}{\partial \nu'} &= 0 \quad \text{on } e_p = \partial T \cap \partial T'. \end{aligned} \tag{2}$$

The continuity of the flux can be weakened as follows:

$$\int_{e_p} \left[K\frac{\partial u}{\partial \nu}\right] = 0$$

and this is the motivation of the CBE method. Introduce F_T, a particular solution of (2) so that

$$F_T(x) = \frac{1}{K_T}\int_T \Gamma(x-y)f(y)dy, \quad x \in T,$$

where $\Gamma(x) = -\frac{1}{2\pi}\log|x|$ is the fundamental solution of $-\Delta$. Then u admits the following decomposition:

$$u = v + (F - H(F)) \quad \text{on } T,$$

where $\Delta v = 0$ and $u = v$ on ∂T. The function $(F - H(F))$ is the Green buuble function.

Our nonconforming CBE method is to find the finite dimensional solution $v_h \in \mathcal{V}_{0,h}$ such that

$$\int_{e_p} \left[K\frac{\partial v_h}{\partial \nu}\right] ds = \int_{e_p} \left[K\left(\frac{\partial H_h(F)}{\partial \nu} - \frac{\partial F}{\partial \nu}\right)\right] ds \quad \text{for all } p \in \mathcal{V}_h^i.$$

Here, H_h is the harmonic interpolation. Then $u_h = v_h + (F - H_h(F))$ is the solution we are looking for.

The advantage of the CBE method is that

1. It derives a naturally flux conserving derivative formulae as the finite volume method.
2. The cost for mesh generation is the same as that of the finite element method.

Therefore, the CBE method can be regarded as an FEM version of the FVM.

Numerical Experiments

The computational domain is taken as the unit square $\overline{\Omega} := [0,1] \times [0,1]$ and a quasi-uniform mesh: the vertices are given as

$$x_i = \frac{2t_i}{1+t_i} \quad \text{and} \quad y_j = \frac{1.5t_j}{1+.5t_j}, \quad 0 \le i,j \le n,$$

where $\{t_j = j/n, j = 0, \cdots, n\}$ and the triangular mesh is then generated by bisecting each rectangle by the diagonal line from the top right to the bottom left.

The P_1 method uses the usual P_1 element, while our $P^*_{2+1/2}$ methods use the following unconventional basis by the nature of our method:

$$\begin{aligned} V_T &= span\{1, x, y, xy, x^2 - y^2, x^3 - 3xy^2\}, \\ \mathcal{V}_h &= \{v_h | v_h \in \oplus_{T \in \mathcal{T}_h} V_T, v_h \text{ is continuous at each node}\}. \end{aligned} \tag{3}$$

Example 1. *We consider the following Poisson equation:*

$$\begin{aligned} -\Delta u &= -4 - 6x \quad \text{in } \Omega, \\ u &= g \quad \text{on } \partial\Omega, \end{aligned}$$

where the function g is chosen so that the exact solution is $u(x,y) = e^x \cos(y) + x^2 + y^2 + x^3$. Then the total flux on $D = [0, 2/3] \times [0, 3/5]$ is 2.4.

n^2	$\|u - u_h\|_{0,h}$	α	$\|\nabla u - \nabla u_h\|_{0,h}$	α	flux
5^2	7.0473e-3		6.3160e-1		
10^2	2.0732e-3	1.7652	3.2263e-1	0.9691	2.4
20^2	5.4437e-4	1.9292	1.6256e-1	0.9889	2.4
40^2	1.3817e-4	1.9781	8.1498e-2	0.9961	2.4

Table 1: Numerical results for the P_1 nonconforming method

n^2	$\|u - u_h\|_{0,h}$	α	$\|\nabla u - \nabla u_h\|_{0,h}$	α	flux
5^2	1.0365e-4		8.9443e-3		
10^2	3.4297e-5	1.5956	2.2992e-3	1.9599	2.4 + 1.57e-4
20^2	9.1723e-6	1.9027	5.7823e-4	1.9914	2.4 + 1.32e-8
40^2	2.3202e-6	1.9830	1.4464e-4	1.9992	2.4 $+\epsilon$

Table 2: Numerical results for the $P^*_{2+1/2}$-method

n^2	$\|u - u_h\|_{0,h}$	α	$\|\nabla u - \nabla u_h\|_{0,h}$	α	flux
5^2	1.5516e-4		9.0081e-3		
10^2	4.5665e-5	1.7646	2.3189e-3	1.9578	2.4
20^2	1.1795e-5	1.9530	5.8307e-4	1.9917	2.4
40^2	2.9673e-6	1.9909	1.4587e-4	1.9990	2.4

Table 3: Numerical results for the modified $P^*_{2+1/2}$-method

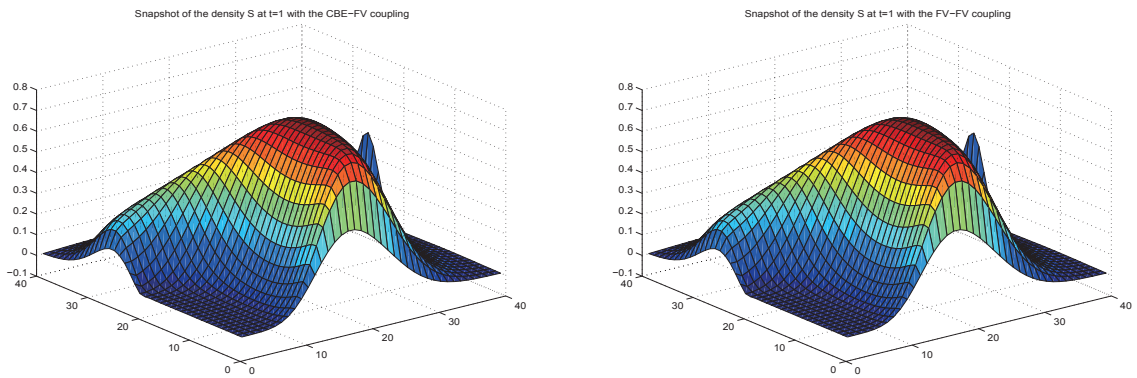

Figure 1: Snapshots of S at $t = 1$ for the P_1 CBE-FV method and FV-FV couplings, respectively

n^2	$\|u - u_h\|_{\infty,h}$	α	$\|\nabla u - \nabla u_h\|_{0,h}$	α
5^2	1.5989e-005		6.8047e-3	
10^2	1.2601e-006	3.6654	1.7463e-3	1.9622
20^2	9.6459e-008	3.7075	4.4266e-4	1.9800
40^2	6.9356e-009	3.7978	1.1146e-4	1.9897

Table 4: Numerical results for the $P_{2+1/2}$-method on the square mesh

Example 2. *We consider a subsurface flow problem.*

$$\begin{aligned} \Delta u &= 1 \quad \text{in } \Omega, \\ \frac{\partial S}{\partial t} &= - \quad \sigma \cdot \nabla S + 0.01 \Delta S \quad \text{in } \Omega, \end{aligned}$$

where $\sigma = -\nabla u$. The boundary condition for u is given as follows:

$$\begin{cases} \frac{\partial u}{\partial \nu} = -1 & \text{on } \{x_1 = 0, \quad 0 < x_2 < 1/2\}, \\ \frac{\partial u}{\partial \nu} = 2 & \text{on } \{x_1 = 1, \quad 1/2 < x_2 < 1\}, \\ u = 0, & \text{elsewhere.} \end{cases}$$

The initial and boundary conditions for S are as follows:

$$S(x,0) = \begin{cases} 1, & x \in (0,1/2) \times (0,1/2), \\ 0, & \text{elsewhere}, \end{cases} \quad \text{and} \quad S(x,t) = 0, \quad x \in \partial\Omega.$$

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New Singular Value Decomposition Algorithm with High Performance

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Singular value decomposition (SVD) of matrices is a basic tool in a very wide area of information processing as a solver for least square problems. A new algorithm with a shift of origin (mdLVs) for computing singular values σ_k of bidiagonal matrices is presented. A shift ${\theta^{(n)}}^2$ is introduced into the recurrence relation

$$\bar{w}_{2k-1}^{(n+1)} = v_{2k-2}^{(n)} + v_{2k-1}^{(n)} - \bar{w}_{2k-2}^{(n+1)} - {\theta^{(n+1)}}^2, \quad \bar{w}_{2k}^{(n+1)} = \frac{v_{2k-1}^{(n)} v_{2k}^{(n)}}{\bar{w}_{2k-1}^{(n+1)}}$$

defined by a discrete-time integrable dynamical system. A shift strategy

$${\theta^{(n)}}^2 = \max\{0, {\vartheta_1^{(n)}}^2 - \varepsilon\}, \quad \vartheta_1^{(n)} := \min_k \left\{ \sqrt{w_{2k-1}^{(n)}} - \frac{1}{2}\left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}} \right) \right\},$$

for any small positive ε, is given so that the singular value computation becomes numerically stable and has a cubic convergence rate and a higher relative accuracy. Therefore the mdLVs algorithm is implemented in DLVS routine which is more accurate and faster than a credible LAPACK routine for singular values.

Secondly, a new double Cholesky factorization of symmetric tridiagonal matrices

$$B^\top B - \left(\frac{1}{\delta^{(0)}} - \frac{1}{\delta^{(\pm 1)}} \right) I = (B^\pm)^\top B^\pm.$$

is also presented by using certain discrete-time integrable systems, which gives rise to a fast algorithm for the associate singular vectors. By taking a suitable $\delta^{(0)}$ we can improve orthogonality of the resulting singular vectors.

A new bidiagonal SVD algorithm (I-SVD) is then designed which is separated into two parts. The first is the mdLVs for accurate singular values. The second part is the double Cholesky factorization. The I-SVD has good properties with respect to both the computational time and the numerical accuracy. The I-SVD algorithm is now implemented in DBDSLV routine which has a better performance with respect to speed, accuracy and scalability than the LAPACK routine for large scaled bidiagonal SVD problem.

Preconditioning and parallelization of I-SVD are also discussed. Combining the algorithm with the block Householder transform and the Murata-Horikoshi-Lang algorithm for bidiagonalization a new fast SVD algorithm for full matrices will be completed.

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A new look at restarted GMRES method*

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ABSTRACT

For a nonsymmetric matrix A, a popular choice for solving the large sparse system of linear equations

$$Ax = b$$

is the famous restarted GMRES algorithm or GMRES(m). However, since GMRES(m) only keeps the the current approximate solution as the new initial guess for the next cycle, restarting would lose most information obtained from the previous cycle of the iteration, the convergence may slow down and even stagnation occurs. Stagnation means that there is no decrease in the residual norm at the end of a restart cycle and is often encountered in the GMRES(m), especially when m is small(but there are exceptions).

After a detailed analysis of occurrence of stagnation of restarted GMRES algorithm, we present a different viewpoint on the implementation of restarted GMRES. Our main idea is that the starting vector at the each restart cycle of GMRES(m) can be chosen flexibly for mitigating occurrence of stagnation or for accelerating the convergence.

Different from usual GMRES(m), the flexibility of choosing the starting vector of the new method provides us a frame work of using inner-outer iterations, in which other iterative methods can be used to get the next starting vector. A simple strategy of taking the harmonic vector associated with the harmonic Ritz value closest to zero as the starting vector is discussed in details. Numerical experiments are done to compare the variant of GMRES(m) combining with this strategy with the original GMRES(m) and demonstrate the former superiority. More precisely, for problems with small eigenvalues well-separated, the numerical experiments show that the new method always outperforms GMRES(m) on moderately restart parameters.

*This is a joint work with Qiang Niu and Michael Ng.

A Rayleigh-Ritz type method for large-scale generalized eigenvalue problems

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1 Introduction

In this paper, we consider a parallel method for computing a limited set of eigenvalues and their corresponding eigenvectors of the generalized eigenvalue problem

$$A\boldsymbol{x} = \lambda B\boldsymbol{x}$$

in a certain region of the complex plane. The generalized eigenvalue problems arise in many scientific and engineering applications. In such applications, the matrices are typically very large, and iterative methods are used to generate a subspace that contain the desired eigenvectors. Approximations are extracted from the subspace through a Rayleigh-Ritz projection. Various methods can be derived from this scheme.

In [4], a moment-based method that finds eigenvalues in a given domain is presented which is based on a root finding method described in [1, 2, 3]. In the method, a small matrix pencil that has only the desired eigenvalues is derived by solving systems of linear equations constructed from A and B. These systems can be solved independently, and we solve them on remote servers using asynchronous remote procedure calls. This approach is suitable for master-worker programming models. A parallel implementation of the method using a GridRPC system and MPI is presented in [5].

Our purpose is to improve numerical stability of the method in [4]. The computation of eigenvalues using explicit moments is sometimes numerically

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unstable. We show that a Rayleigh-Ritz procedure can be used to avoid the use of explicit moments.

2 A Rayleigh-Ritz type method

We apply a Rayleigh-Ritz procedure with an orthogonal basis Z_m. The projected matrices are given by $A_m = Z_m^H A Z_m$ and $B_m = Z_m^H B Z_m$. The Ritz values of the projected pencil (A_m, B_m) are taken as approximate eigenvalues for the original pencil (A, B) with corresponding Ritz vectors. We can derive various methods by a choice of Z_m.

Let Γ be a circle with radius γ centered at ρ. Suppose that m distinct eigenvalues $\lambda_1, \ldots, \lambda_m$ are located inside Γ. For a nonzero vector $\boldsymbol{v} \in \mathbb{R}^n$, we define

$$\boldsymbol{m}_k := \frac{1}{2\pi \mathrm{i}} \int_\Gamma (z-\gamma)^k (zB - A)^{-1} \boldsymbol{v} dz, \quad k = 0, 1, \ldots, m-1.$$

If $Z_m \in \mathrm{span}(\boldsymbol{m}_0, \ldots, \boldsymbol{m}_{m-1})$, then the Ritz values are just $\lambda_1, \ldots, \lambda_m$. This implies that the eigenvalues located inside Γ can be obtained with vectors obtained by the contour integral.

By approximating the contour integral via the N-point trapezoidal rule, we obtain the following approximations for $\boldsymbol{m}_k$:

$$\boldsymbol{m}_k \approx \hat{\boldsymbol{m}}_k := \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} (\omega_j B - A)^{-1} \boldsymbol{v}, \quad k = 0, 1, \ldots m-1,$$

where N is a positive integer, and

$$\omega_j = \gamma + \rho e^{\frac{2\pi \mathrm{i}}{N}(j+1/2)}, \quad j = 0, 1, \ldots, N-1.$$

In the computation of $\hat{\boldsymbol{m}}_k$, we solve a number of systems of linear equations. When the matrices A and B are large, the computational costs to solve these systems are dominant in the algorithm. Since these linear systems are independent on each ω_j, we solve them on remote servers in parallel. This process derives a master-worker type parallel method.

We have implemented the proposed method combining a GridRPC system and MPI. We report the performance of the application of the proposed method on PC clusters that were used over a wide-area network.

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Iterative Splitting Methods for Nonsymmetric Algebraic Riccati Equations

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We study numerical solution of the nonsymmetric *algebraic Riccati equation* (ARE)

$$\mathcal{R}(X) = XCX - XD - AX + B = 0, \tag{1}$$

where A, B, C and D are real matrices of sizes $m \times m$, $m \times n$, $n \times m$ and $n \times n$, respectively.

ARE(1) may arise in many areas of scientific computing and engineering applications such as the total least squares (TLS) problems with or without symmetric constraints [3], the spectral factorizations of rational matrix functions [2, 5], the linear and nonlinear optimal controls [18, 21], the constractive rational matrix functions [14, 6], the structured stability radius [11], the transport theory [13], the Wiener-Hopf factorization of Markov chains [22], the computation of matrix sign function [19, 16] and the optimal solutions of linear differential systems [15].

There are many studies about theoretical properties and numerical algorithms for ARE(1) as well as its special cases, see [4, 17, 20] and references therein. To compute the minimal positive solution of ARE(1) under certain assumptions, Guo and Laub [9] recently established and studied the following Newton iteration method and fixed-point iteration method:

The Newton and The Fixed-Point Iteration Methods.
`Set` $X_0 = 0 \in \mathbb{R}^{m\times n}$. `For` $k = 0, 1, 2, \ldots$ `until the matrix sequence` $\{X_k\}$ `convergence, compute` X_{k+1} `from` X_k `by solving the Sylvester equation`

$$(A - X_kC)X_{k+1} + X_{k+1}(D - CX_k) = B - X_kCX_k, \quad \texttt{for Newton iteration}, \tag{2}$$

`or`

$$M_AX_{k+1} + X_{k+1}M_D = N_AX_k + X_kN_D + X_kCX_k + B, \quad \texttt{for fixed-point iteration}. \tag{3}$$

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Here, $A = M_A - N_A$ and $D = M_D - N_D$ are prescribed splittings of the matrices A and D, respectively.

Let

$$W = I \otimes A + D^T \otimes I.$$

Then Guo and Laub proved in [9] that ARE(1) has at least a positive solution when the matrices A, B, C and D satisfy the assumption:

(A_1) $B > 0$, $C > 0$ and W is a nonsingular M-matrix.

Moreover, they showed that both the Newton and the fixed-point iterations monotonically increasingly converge to the minimal positive solution of ARE(1), provided for the fixed-point iteration the involved splitting matrices satisfy that M_A and M_D are Z-matrices and N_A and N_D are nonnegative matrices. In particular, they verified that ARE(1) arising from the transport theory automatically satisfy assumption (A_1), see also [12, 13]. Latter, in [8] Guo further relaxed assumption (A_1) to the following:

(A_2) $B \geq 0$, $C \geq 0$ and W is a nonsingular M-matrix,

or sometimes (A_2) and

(A_3) $B \neq 0$, $C \neq 0$ and $W^{-1} \cdot \mathrm{vec}(B) > 0$,

and proved the following results:

(i) when assumptions (A_2) and (A_3) are satisfied, if there exists a positive matrix X_f such that $\mathcal{R}(X_f) \leq 0$, then ARE(1) has a minimal positive solution S such that $S \leq X_f$ and the Newton iteration starting from $X_0 = 0$ converges to S monotonically increasingly and quadratically; and

(ii) when assumption (A_2) is satisfied, if there exists a positive matrix X_f such that $\mathcal{R}(X_f) \leq 0$, then ARE(1) has a minimal positive solution S such that $S \leq X_f$ and the fixed-point iteration starting from $X_0 = 0$ converges to S monotonically increasingly and linearly, provided that the splitting matrices M_A and M_D are Z-matrices and N_A and N_D are nonnegative matrices.

In addition, he derived a sufficient and necessary condition for guaranteeing the existence of the minimal nonnegative solution S of ARE(1), and described a Schur factorization method for computing the S.

More recently, Guo and Bai [10] gave the sensitivity analysis of the minimal nonnegative solution of ARE(1) and described a matrix sign function method for computing this solution.

However, either the Newton iteration method or the fixed-point iteration method requires solving a Sylvester equation at each step of the iterations. This is very costly and complicated in actual applications, in particular, when the matrix sizes are very large, although several feasible and efficient Sylvester-equation solvers, e.g., the Bartels-Stewart method [1] and the Hessenberg-Schur method [7], are available.

In this talk, we establish a class of *alternately linearized implicit* **(ALI)** iteration methods for solving the minimal nonnegative solutions of the nonsymmetric algebraic Riccati equations (1) based on technical combination of alternate splitting and successive approximating of the algebraic Riccati operators. These methods include one iteration parameter, and suitable choices of this parameter may result in fast convergent iteration methods; and they only involve matrix operations and are, hence, more convenient for being implemented in parallel computing environments. Under suitable nonnegativity and monotonicity assumptions about the involved matrices A, B, C and D, we prove the monotone convergence and estimate the asymptotic convergence factor of the ALI iteration matrix sequences. Numerical experiments show that the ALI iteration methods are feasible and effective, and can outperform the Newton iteration method and the fixed-point iteration methods. Besides, we further generalize the known fixed-point iterations discussed in [9], obtaining an extensive class of relaxed splitting iteration methods, such as the SOR-type fixed point iteration and the AOR-type fixed point iteration [1] as well as their blockwise variants, for solving the nonsymmetric algebraic Riccati equations (1).

We remark that for ALI iteration method the choice of a practically optimal parameter is often problem-dependent and, therefore, is considerably difficult in the viewpoints of both theory and application. This is equally true for the SORFP and the AORFP iteration methods.

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A Posteriori Error Analysis and Adaptive Methods for Partial Differential Equations

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Abstract. The adaptive finite element method based on a posteriori error estimates provides a systematic way to refine or coarsen the meshes according to the local a posteriori error estimator on the elements. One of the remarkable properties of the method is that for appropriately designed adaptive finite element procedures, the meshes and the associated numerical complexity are quasi-optimal in the sense that in two space dimensions, the finite element discretization error is proportional to $N^{-1/2}$ in terms of the energy norm, where N is the number of elements of the underlying mesh. The purpose of this talk is to report some of the recent advances in the a posteriori error analysis and adaptive finite element methods for partial differential equations.

We consider to use AFEM to solve the Helmholtz-type scattering problems with perfectly conducting boundary

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbf{R}^2 \backslash \bar{D}, \tag{0.1a}$$

$$\frac{\partial u}{\partial \mathbf{n}} = -g \quad \text{on } \Gamma_D, \tag{0.1b}$$

$$\sqrt{r}\left(\frac{\partial u}{\partial r} - \mathbf{i}ku\right) \to 0 \quad \text{as } r = |x| \to \infty. \tag{0.1c}$$

Here $D \subset \mathbf{R}^2$ is a bounded domain with Lipschitz boundary Γ_D, $g \in H^{-1/2}(\Gamma_D)$ is determined by the incoming wave, and $\mathbf{n}$ is the unit outer normal to Γ_D. We assume the wave number $k \in \mathbb{R}$ is a constant. We study an *adaptive perfectly matched layer* (APML) technique to deal with the Sommerfeld radiation condition (0.1c) in which the PML parameters such as the thickness of the layer and the fictitious medium property are determined through sharp a posteriori error estimates. The APML technique combined with AFEM provides a complete numerical method for solving the scattering problem in the framework of finite element which has the nice property that the total computational costs are insensitive to the thickness of the PML absorbing layers. The quasi-optimality of underlying FEM meshes is also observed.

Things become much more complicated when applying AFEM to solve time-dependent partial differential equations. One important question is if one should use the *adaptive method of lines* (AML) in which variable timestep sizes (but constant at each time step) and variable space meshes at different time steps are assumed, or one should consider the the *space-time adaptive method* in which space-time domain is considered as a whole and AFEM is used without distinguishing the difference of time and space variables. Our recent studies in [2, 3, 4] reveal that with sharp a posteriori error analysis and carefully

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designed adaptive algorithms, the AML method produces the very desirable quasi-optimal decay of the error with respect to the computational complexity

$$|||u - U|||_{\Omega\times(0,T)} \leq CM^{-1/3} \tag{0.2}$$

for a large class of convection-diffusion parabolic problems in two space dimensions using backward Euler scheme in time and conforming piecewise linear finite elements in space. Here $|||u-U|||_{\Omega\times(0,T)}$ is the energy norm of the error between the exact solution u and the discrete solution U, and M is the sum of the number of elements of the space meshes over all time steps. Thus if one takes the quasi-optimality of the computational complexity as the criterion to assess the adaptive methods, then the space-time adaptive method which is less studied in the literature will not have much advantage over the AML method.

A posteriori error analysis for parabolic problems in the framework of AML has been studied intensively in the literature. The main tool in deriving a posteriori error estimates in [7, 8, 6, 9, 1] is the analysis of linear dual problems of the corresponding *error* equations. The derived a posteriori error estimates, however, depend on the H^2 regularity assumption on the underlying elliptic operator. Without using this regularity assumption, energy method is used in [10, 2] to derive an a posteriori error estimate for the total energy error of the approximate solution for linear heat equations. A lower bound for the local error is also derived for the associated a posteriori error indicator in [10, 2]. In [2] an adaptive algorithm is constructed which at each time step, is able to reduce the error indicators (and thus the error) below any given tolerance within finite number of iteration steps. Moreover, the adaptive algorithm is quasi-optimal in terms of energy norm. In [3] an quasi-optimal AML method in terms of the energy norm is constructed for the linear convection-dominated diffusion problems based on L^1 a posteriori error estimates.

We study the AML method for the initial boundary value problems of nonlinear convection-diffusion equations of the form

$$\frac{\partial u}{\partial t} + \mathrm{div} f(u) - \Delta A(u) = g.$$

We derive sharp $L^\infty(L^1)$ a posteriori error estimates under the non-degeneracy assumption $A'(s) > 0$ for any $s \in \mathbf{R}$. The problem displays both parabolic and hyperbolic behavior in a way that depends on the solution itself. It is discretized implicitly in time via the method of characteristic and in space via continuous piecewise linear finite elements. The analysis is based on the Kružkov "doubling of variables" device and the recently introduced "boundary layer sequence" technique to derive the entropy error inequality on bounded domains. The derived a posteriori error estimate leads to a quasi-optimal adaptive method in terms of the $L^\infty(L^1)$ norm of the error.

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The Finite Element Methods dealing with Domain Singularities

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Solutions of elliptic boundary value problems on a domain with corners have singular behavior near the corners. This occurs even when data of the underlying problem are very smooth. Such singular behavior affects the accuracy of the finite element method throughout the whole domain. We are concerned about the cure of this phenomenon.

We consider two Model problems;

The first one is the Poisson equation;

(1) The Poisson equation with the Dirichlet boundary condition in a non-convex polygon $\Omega \in R^2$:

$$\begin{cases} -\Delta u &= f, \quad \text{in } \Omega, \\ u &= 0, \quad \text{on } \partial\Omega, \end{cases} \tag{0.1}$$

where Δ stands for the Laplacian operator, f is a given function in $L^2(\Omega)$, and Ω is an open, bounded polygonal domain in R^2.(For simplicity assume Ω have only one re-entrant angle.)

The second one is the Interface Problem;

(2) Let Ω_j ($j = 1, ..., J$) be open, polygonal subdomains of Ω:

$$\Omega_i \cap \Omega_j = \emptyset \quad \text{for } i \neq j \quad \text{and} \quad \bigcup_{j=1}^{J} \bar{\Omega}_j = \bar{\Omega}.$$

The Model interface problem is: find $u \in H_0^1(\Omega)$ such that

$$-\mathrm{a}_j \, \Delta u = f \quad \text{in } \Omega_j \tag{0.2}$$

for $j = 1, \dots, J$ with interface conditions

$$\mathrm{a}_i \frac{\partial u}{\partial \mathbf{n}_i}|_{\Gamma_{ij}} + \mathrm{a}_j \frac{\partial u}{\partial \mathbf{n}_j}|_{\Gamma_{ij}} = 0 \tag{0.3}$$

for $i, j = 1, \dots, J$ such that $\Gamma_{ij} \neq \emptyset$. Denote by $\Gamma_{ij} = \partial\Omega_i \cap \partial\Omega_j$ the common edge of Ω_i and Ω_j and let $\mathbf{n}_j$ be the outward unit normal vector to the boundary $\partial\Omega_j$ of

Ω_j. Assume that the diffusion coefficient a is piecewise constant with respect to the partition:

$$\mathrm{a}(x) = \mathrm{a}_j > 0 \quad \text{in } \Omega_j \tag{0.4}$$

for $j = 1, \ldots, J$.

We developed a new finite element method for the Poisson equations (0.1) with homogeneous Dirichlet boundary conditions on a polygonal domain with one re-entrant angle. It is well-known that the solution of such problem has a singular representation: $u = w + \lambda\eta s$ where $w \in H^2(\Omega) \cap H_0^1(\Omega)$, $\lambda \in R$ and η are the respective stress intensity factor and cut-off function, and s is a known singular function depending only on the re-entrant angle. By using the dual singular and an extra cut-off functions, we are able to deduce a well-posed variational problem for w and an extraction formula for λ in terms of w. Standard continuous piecewise linear finite element approximation yields $O(h)$ and $O(h^{1+\frac{\pi}{\omega}-\epsilon})$ accuracy for w in the respective H^1 and L^2 norms, where ω is the internal angle and ϵ is any positive number. These, in turn, imply $O(h^{1+\frac{\pi}{\omega}-\epsilon})$ approximation for λ in the absolute value and $O(h)$ and $O(h^{1+\frac{\pi}{\omega}-\epsilon})$ approximation for u in the repective H^1 and L^2 norms(see [1, 2, 3]). This method can be regarded as a kind of SFM.

Now we applied this new SFM to the interface problem (0.2).

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High-Accurate Numerical Computation with Multiple-precision Arithmetic and Spectral Method

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We propose the use of multiple-precision arithmetic and high-accurate discretizations for numerical computations of ill-posed or unstable problems. Two different kinds of computational errors are considered in the research: discretization errors which come from the discretization of differential or integral operators, and rounding errors which are included in the discretization of real numbers and their arithmetic. Rounding errors are not matter in stable numerical method. In numerically unstable processes rounding error is artificial high-frequency disturbance and its rapid growth is crucial.

Numerically unstable processes appear in numerical method of inverse problems which are important in engineering, geophysics or medicine as non-destructive tests, computer tomography or remote sensing. They are ill-posed in the sense of Hadamard in most cases, especially instability breaks their direct numerical method. We define a problem is well-posed in the sense of Hadamard if and only if there exists a unique solution and it continuously depends on data. Ill-posedness is the opposite concept to well-posedness and instability is most defect in numerical analysis because it leads the rapid growth of errors in numerical processes. We give a remark that unstable process arises from mathematically stable problems.

Stability is one of the most important issues in numerical analysis. Mathematical stability of a partial differential equation or an integral equation usually derives stability of its discretization scheme, however, stability of its numerical processes is not derived straightforwardly. In other words, numerical implementation of the mathematically stable scheme may be unstable. For example Tikhonov regularized equation [11] is mathematically well-posed and stable for any regularization parameters, however its numerical process becomes unstable for small regularization parameters. Stability of numerical processes depends on the each computational environments including user programs statements, approximation of real numbers, and its precision.

To discuss precisely we denote the problem as

$$Au = f, \tag{1}$$

and its discretization scheme as

$$A_h u_h = f_h, \tag{2}$$

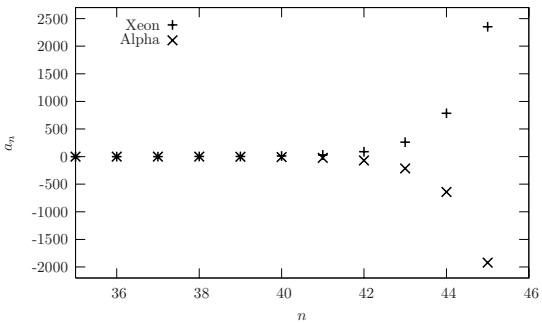
where h denotes discretization parameters. In numerical computation, we intend to implement (2) on digital computers. However the equation (2) contains real numbers and exact arithmetic then we can not obtain the exact values u_h in numerical computations with computer arithmetic. We consider a relation

$$A_{h,p} u_{h,p} \approx f_{h,p} \tag{3}$$

as numerical process of (2), where we denote p to show numerical results $u_{h,p}$ depend on a program and precision of arithmetic. We obtain $u_{h,p}$ as numerical results which approximates the exact solution u_h of (2), and differences between u_h and $u_{h,p}$ are caused by rounding errors. Even if (1) or (2) is mathematically stable, its implementation (3) is possibly unstable processes. For example, let us consider a recursion formula

$$a_{n+2} = \frac{34}{11} a_{n+1} - \frac{3}{11} a_n, \qquad n = 0, 1, 2, 3, \cdots, N. \tag{4}$$

The exact solution of (4) is $a_n = c_1(1/11)^n + c_2 3^n$, where c_1 and c_2 are linear combinations of the initial values a_0 and a_1, and a_N continuously depends on a_0 and a_1 for a fixed N. However its numerical processes is unstable because the solution contains an exponentially growing term 3^n. Indeed for $a_0 = 1, a_1 = 1/11$, we obtain different solutions $\{a_n\}$ on different computers shown in Figure 1, and both solutions diverge and do not approximate the exact solutions $a_n = (1/11)^n$. On the other hand we obtain good numerical



n	Xeon (Linux,gcc)	Alpha (Linux,gcc)
2	0 00826446	0 00826446
5	$6\ 20921 \times 10^{-6}$	$6\ 20921 \times 10^{-6}$
10	$3\ 86014 \times 10^{-11}$	$3\ 85159 \times 10^{-11}$
40	9 68369	$-7\ 91327$
50	571812	-467270

Figure 1: Numerically Unstable Processes for Recursion Formula (4)

solutions with multiple-precision arithmetic. The result shows that stability of numerical processes depends on arithmetic precision in the processes.

In the standard numerical computation the real numbers and their arithmetic are discretized with IEEE754 standard [7], in which real number is approximated with a floating-point number [9, 5] which consists of a sign part, a exponent part, and a fraction part. IEEE754 double is most widely used today, and it have about 15 digits accuracy in its fractional part. Multiple-precision arithmetic is one of the ways to extend the fractional digits to improve accuracy of approximation of real numbers. Because rounding errors are quite artificial disturbance qualitative approaches like stability analysis or stabilization techniques are sometimes not effective for evaluation of numerical results. We propose quantitative a posteriori approach with interval arithmetic with multiple-precision to analyze the influence of rounding errors.

Multiple-precision arithmetic is expensive in both time and memory costs for large scale problems. For a request of fast computing we implement a new multiple-precision arithmetic [2] which works with the programming language C++ or Fortran90. It runs on personal computers, clusters, or supercomputers with parallel computation.

We must also reduce discretization error for unstable problems. Spectral methods [1, 6] give high-accurate discretization manners. For integral equations of the first kind with analytic kernel, Chebyshev spectral methods are applied and realize numerical simulations [8, 3]. For partial differential equations spectral collocation patch method or spectral element method [10] are known as a high-accurate numerical method for the purpose of direct numerical computation of unstable problems.

From a view point of inverse problems, stabilization such as Tikhonov regularization is effective to hide the influence of various errors. On the other hand strong stabilizations hide important characteristics like singularities of solutions and problems at the same time. The balance of mathematical stabilization technique is important [4].High-accurate numerical method is required for precise numerical analysis with stabilization techniques.

In the talk, we shall introduce our multiple-precision arithmetic computation environment and show some numerical examples with the proposed environment.

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A NEUMANN-DIRICHLET PRECONDITIONER FOR A FETI-DP FORMULATION WITH MORTAR METHODS

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This talk is concerned with a preconditioner for an iterative method for the parallel solution of the elliptic problem, the two-dimensional Stokes problem and the three-dimensional compressible elasticity problem with nonconforming discretizations. Of the many methods for nonmatching meshes, including [4] and [16], we consider the mortar method [1, 3, 18, 19].

Recently the dual-primal FETI (FETI-DP) method introduced by Farhat, Lesoinne, and Pierson [7] has been applied to mortar finite elements methods [5, 6, 17]. For FETI-DP methods on nonmatching grids, Dryja and Widlund [5] proposed a preconditioner, so-called Dirichlet preconditioner, which gives a condition number bound $C(1+\log(H/h))^2$ with the Neumann–Dirichlet ordering of substructures, where H and h denote the maximum diameter of subdomains and the minimum size of meshes of all subdomains, respectively. Moreover, in [6], they proposed a different preconditioner, which is similar to one in [12], and proved the condition number bound $C(1+\log(H/h))^2$. However, the constant C in the condition number bound depends on the ratio of meshes between neighboring subdomains. This restriction is impractical when the coefficients of elliptic problems are highly discontinuous between subdomains (see Wohlmuth [19]).

In [10], a FETI-DP operator was formulated in a different way from that of Dryja and Widlund [5, 6] and a Neumann–Dirichlet preconditioner was proposed, which gives the condition number bound $C \max_{i=1,\cdots,N} \left\{ (1+\log(H_i/h_i))^2 \right\}$ with the constant C not depending on the ratio of meshes between neighboring subdomains. The proposed preconditioner is similar to the previous FETI-DP preconditioners except that it solves local problems with Neumann boundary conditions on nonmortar interfaces and with a zero Dirichlet boundary condition on mortar interfaces. The additional complication caused by mortar discretizations can be handled by using this preconditioner.

The extension of the FETI-DP method in [10] has been done to the three dimensional problem [8]. In the FETI-DP formulation, we need redundant continuity constraints to get the same condition number bound as the two dimensional problem. The redundant constraints are that averages of the solution across subdomain interfaces are the same, which is so called face constraints in [14]. With the similar idea to the previous work in [10], a Neumann-Dirichlet preconditioner is proposed, and it is shown that the same condition number bound as the two-dimensional elliptic problem holds for the three-dimensional elliptic problems whose coefficients do not change rapidly across subdomain interfaces. Further, with an assumption on mesh sizes according to the magnitude of coefficients, we get the same condition number bound for elliptic problems with discontinuous constant coefficients. In this case, the constant C does not depend on the coefficients.

In [11] the FETI-DP algorithm developed in [10] was extended to the two-dimensional Stokes problem. The inf-sup stable $P_1(h) - P_0(2h)$ finite element space is considered in each subdomain. The mortar matching conditions are imposed on the velocity functions. An optimal approximation of mortar methods for the Stokes problem was proved by Belgacem [2]. If the inf-sup constant is independent of mesh sizes and

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subdomain sizes, then the optimal order of approximation follows independently of the number of subdomains and mesh sizes as in the case of elliptic problems. As in [8, 15], the primal constraints, i.e., edge average and vertex constraints, are introduced to solve the Stokes problem efficiently and correctly. Then a Neumann-Dirichlet preconditioner is proposed and the same condition number bound is analyzed.

The FETI-DP algorithm of [10] was extended to the three-dimensional compressible elasticity problem [9]. Klawonn and Widlund [13] considered various primal constraints for elasticity problems with discontinuous Lamé parameters. In their work, some faces and edges are selected as fully primal faces and fully primal edges. They work with edge average constraints on a fully primal face, and edge average and edge moment constraints on a fully primal edge. However, edge constraints are not compatible with mortar matching constraints. In [9], the face average and face moment constraints on the faces are introduced. Further, the number of primal constraints are reduced by selecting only some of the faces as primal faces for which the face average and face moment constraints are applied.

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Numerical verification methods of bifurcating solutions for two- and three-dimensional Rayleigh-Bénard problems

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Abstract

The Rayleigh-Bénard heat convection problems are approximated by the Oberbeck–Boussinesq equations on the unbounded horizontal domain to find $\mathbf{u}$ the velocity field, p the pressure and T the temperature of the fluid satisfying the followings:

$$\rho_0 \left[\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] + \nabla p = \mu\Delta\mathbf{u} - \rho g \mathbf{e}_3, \quad (1)$$

$$\rho_0 C_p \left[T_t + (\mathbf{u}\cdot\nabla)T\right] = k\Delta T, \quad (2)$$

where ρ_0 is a reference density, μ dynamic viscosity, g gravity acceleration, $\mathbf{e}_i$ unit vector along x_i direction, C_p specific heat at constant pressure, and k thermal conductivity. And the density ρ depends on T: $\rho = \rho(T) = \rho_0[1 - \alpha_T(T - T_0)]$ with thermal expansion coefficient α_T and temperature T_0 on the top. We consider the numerical verification method for stationary solutions of equations (1) and (2) in two and three space dimensions. Under some appropriate boundary conditions, based on a Fourier spectral method and the constructive error estimates, we succeeded to verify numerically several nontrivial solutions which are bifurcating from trivial solutions near the critical Rayleigh number as well as the bifurcation point itself. Numerical examples will be presented in the talk.

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