

2024年秋季 · 多层迭代法 课程内容总结



日期: 2024.11.28

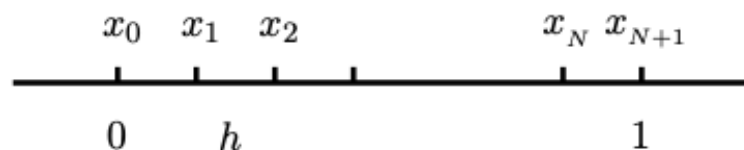


教师: 张晨松, 中国科学院数学与系统科学研究院

模型问题：求解Poisson方程

模型方程及其有限差分离散：

$$\begin{aligned} -u''(x) &= f, & x \in (0, 1) \\ u(x) &= 0, & x = 0, 1 \end{aligned}$$



$$\begin{aligned} u''(x_j) &= \frac{1}{h^2} \left[u(x_{j-1}) - 2u(x_j) + u(x_{j+1}) \right] + O(h^2) \\ &\approx \frac{1}{h^2} \left[u_{j-1} - 2u_j + u_{j+1} \right], \end{aligned}$$

$$\vec{f} := \left(f_j \right)_{j=1}^N = \left(f(x_j) \right)_{j=1}^N$$

问题特点：

- 常用模型问题：方程足够简单，但包含了很多重要应用的难点特征
- 应用范围广泛：Heat conduction, fluid flow, porous-media flow,
- 问题条件数大：条件数随网格尺寸平分反比增长, ill-conditioned
- 实际应用问题：**各向异性**、**跳跃系数**、**非均质性**、.....

可用方法：

- 追赶法, LU
- FFT
- CG
- **Multigrid**

简单迭代法的主要思想

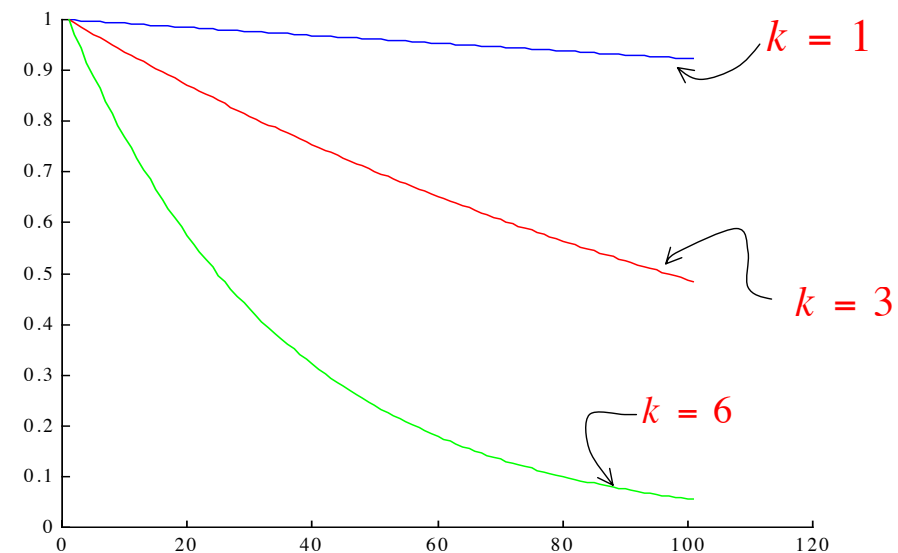
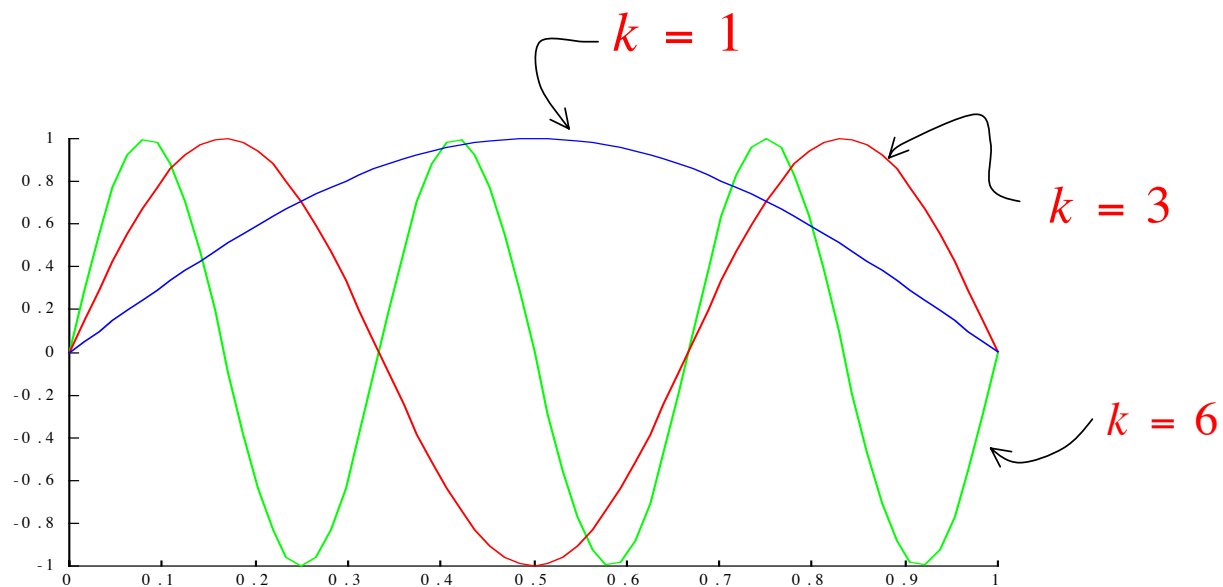
Algorithm 1: Iterative solver

```
1 %% Given a nonsingular matrix  $A \in \mathbb{R}^{n \times n}$ ,  $b \in \mathbb{R}^n$ , and an initial guess  $x_0 \in \mathbb{R}^n$ ;  
2 for  $i = 0$  : MaxIter or converged  
3     Compute  $r_i \leftarrow b - Ax_i$ ;  
4     Solve the error equation  $Ae_i = r_i$  approximately;  
5     Update  $x_{i+1} \leftarrow x_i + e_i$ ;  
6 end
```

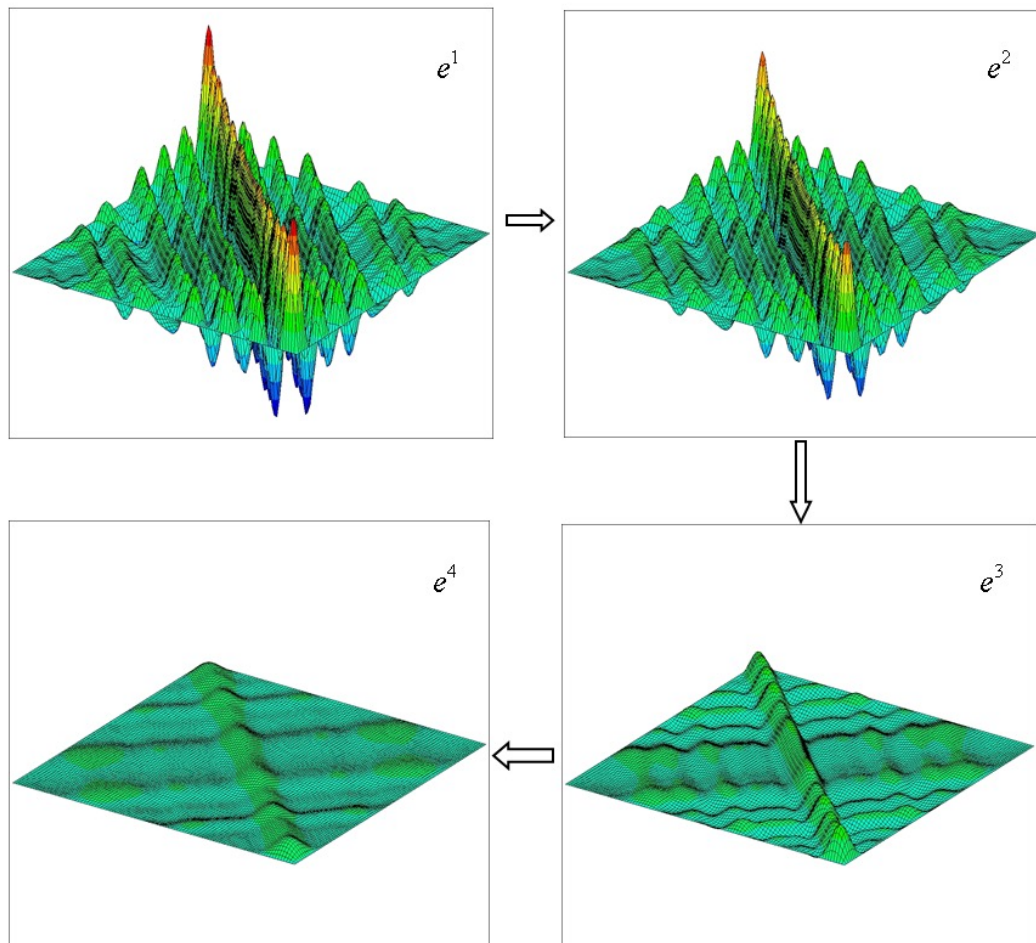
简单迭代:

$$x \leftarrow x + S(b - Ax)$$

- wJacobi或GS方法等
- 程序非常简单
- 收敛速度极慢



两层网格法的主要思想



仅使用磨光算法的效果

两层网格方法 (TG) :

- Step 1. 前磨光 (简单迭代法)

$$x \leftarrow x + S(b - Ax)$$

- Step 2. 粗空间校正 (CGC)

$$x \leftarrow x + PA_c^{-1}R(b - Ax)$$

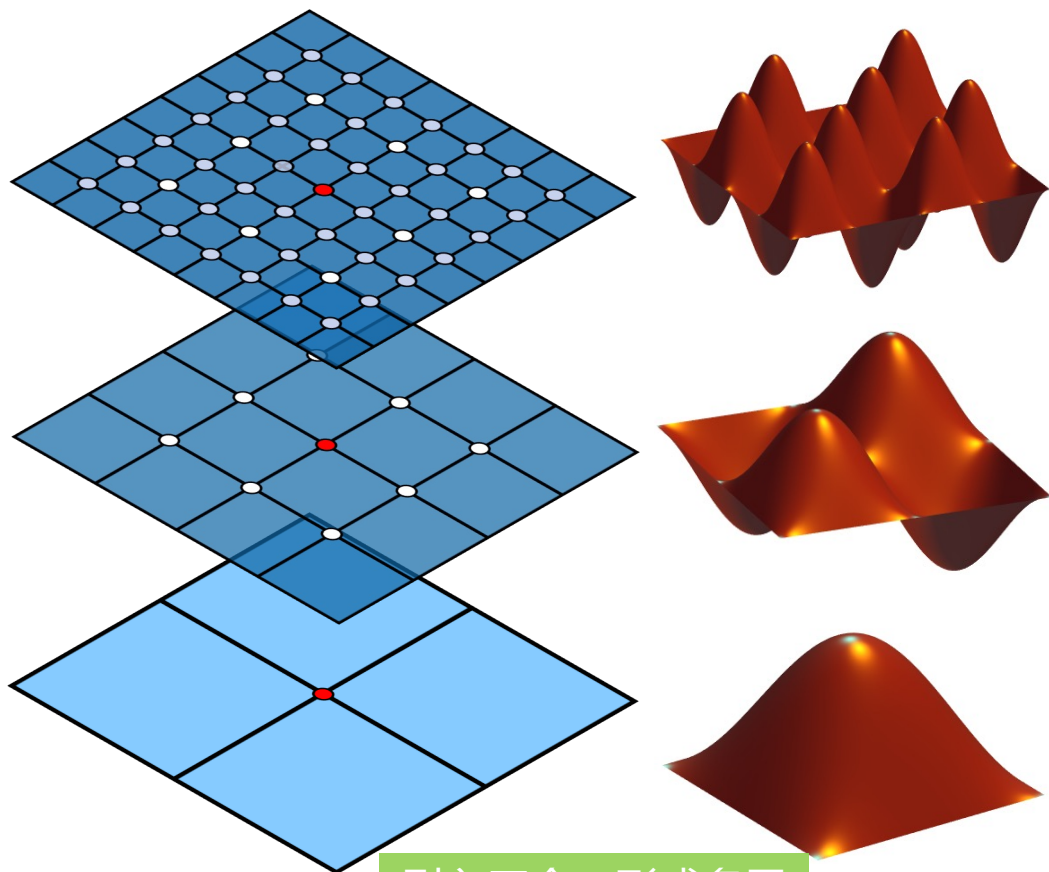
两层网格方法误差传播算子:

$$\begin{aligned} E_{TG} &= (I - \Pi_c)(I - SA) \\ &= (I - PA_c^{-1}RA)(I - SA) \end{aligned}$$

利用磨光消除高频误差, 利用粗网格校正CGC消除低频误差

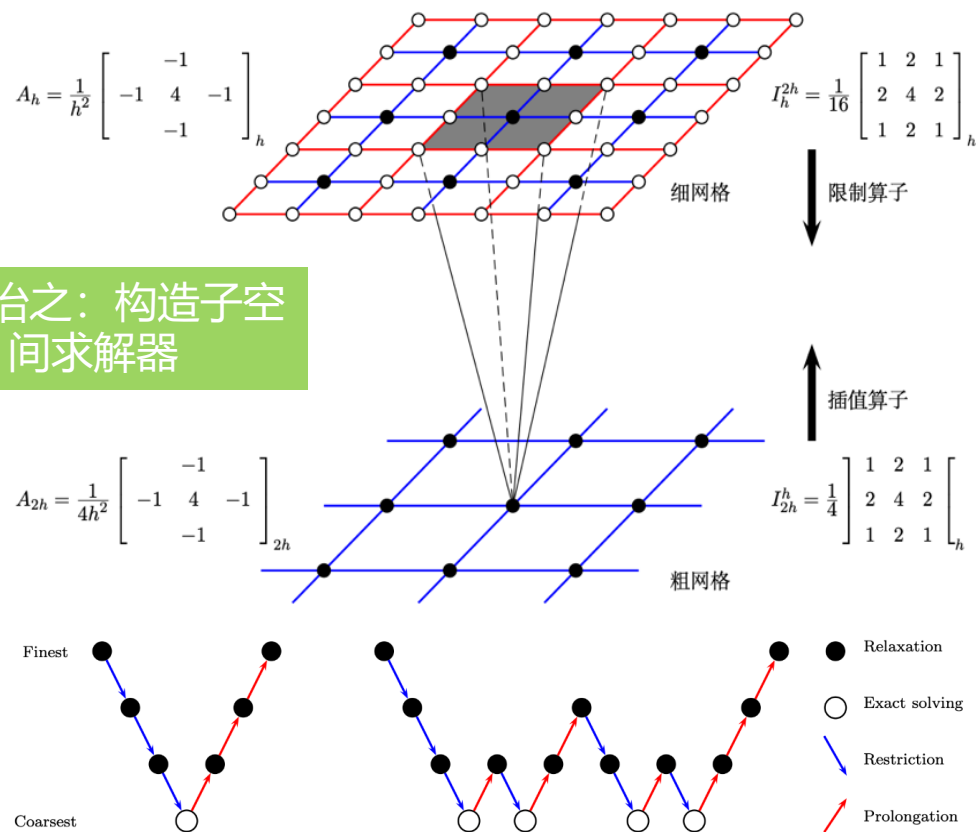
多层迭代法的主要思路

问题：如何处理低频误差分量？如何有效消除全局误差的影响？如何高效地进行实现？



引入冗余：形成多层子空间分解

分而治之：构造子空间求解器



分层迭代：有效的嵌套迭代格式

多层网格v-循环伪代码

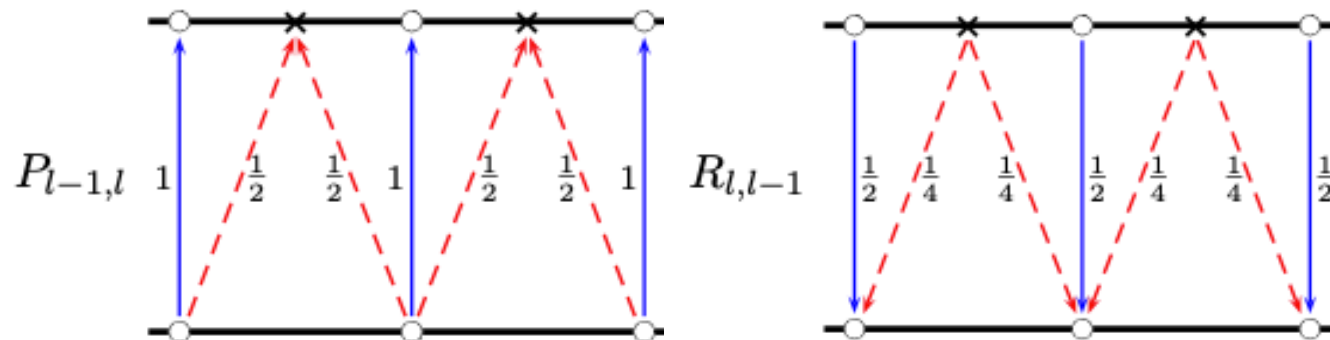
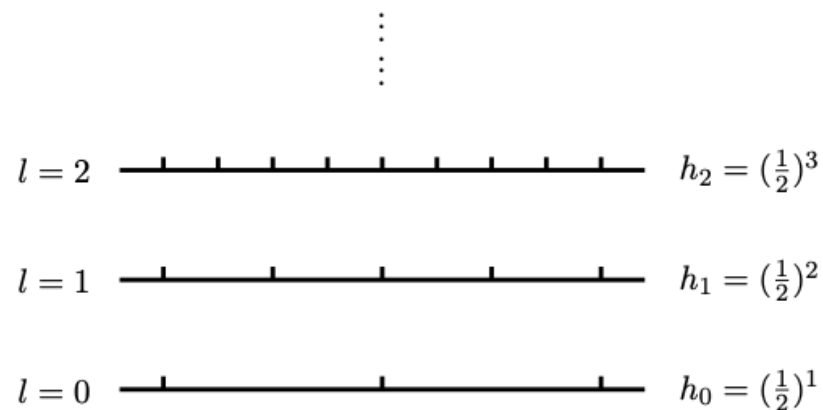
```
1  %% For any level  $\ell$ , give a nonsingular matrix  $A_\ell$  and prolongation  $P_\ell$ ;  
2  %% Compute the residual  $r_\ell$  of the current iteration;  
3   $x_\ell \leftarrow Sr_\ell$ ; %% pre-smoothing  
4  if  $\ell > 0$  %% not the coarsest level yet  
5       $r_\ell \leftarrow r_\ell - Ax_\ell$ ; %% form residual  
6       $r_{\ell-1} \leftarrow P_\ell^T r_\ell$ ; %% restriction  
7       $e_{\ell-1} \leftarrow V(A_{\ell-1}, r_{\ell-1}, P_{\ell-1}, \ell - 1)$ ; %% recursive call  
8       $e_\ell \leftarrow P_\ell e_{\ell-1}$ ; %% prolongation  
9       $x_\ell \leftarrow x_\ell + e_\ell$ ; %% correction  
10      $r_\ell \leftarrow r_\ell + Ae_\ell$ ; %% update residual (optional)  
11      $x_\ell \leftarrow x_\ell + S^T r_\ell$ ; %% post-smoothing (optional)  
12 end  
13 return  $x_\ell$ 
```

简单示例：1D几何多层网格法

1D Poisson方程的GMG:

- FDM五点差分模板
- 需要层次化结构网格
- 可采用无矩阵实现方法，效率高

$$A = \frac{1}{h^2} \text{tridiag}(-1, 2, -1), \quad f_i = f(x_i).$$



$$P_{l-1,l} := \frac{1}{2} \begin{pmatrix} \dots & & & & & & & & \\ & 1 & & & & & & & \\ & 2 & & & & & & & \\ & 1 & 1 & & & & & & \\ & & 2 & & & & & & \\ & & & 1 & & & & & \\ & & & & 1 & & & & \\ & & & & & \dots & & & \end{pmatrix} \quad R_{l,l-1} := \frac{1}{4} \begin{pmatrix} \dots & & & & & & & & \\ & 1 & 2 & 1 & & & & & \\ & & & 1 & 2 & 1 & & & \\ & & & & & & \dots & & \end{pmatrix}$$

粗网格问题: $A_c = \left(\frac{h}{H} P^T \right) A P =: R A P.$

或可直接由粗网格进行离散获得

多层网格法的简单示例

I need a geometric multigrid solver for the Poisson's equation in 2D. Can you write a MATLAB code for me?

```
1 function gmg_poisson_2d()
2     % Grid parameters
3     n = 64; % Number of grid points (must be power of 2)
4     L = 1; % Length of the domain
5     h = L / (n - 1); % Grid spacing
6
7     % Generate grid
8     [x, y] = meshgrid(0:h:L, 0:h:L);
9
10    % Define the right-hand side
11    f = sin(pi * x) .* sin(pi * y);
12
13    % Initial guess
14    u = zeros(size(f));
15
16    % Solve using GMG
17    num_cycles = 10; % Number of V-cycles
18    u = v_cycle(u, f, h, num_cycles);
19
20    % Plot solution
21    figure;
22    surf(x, y, u, 'EdgeColor', 'none');
23    title('Solution to Poisson Equation');
24    xlabel('x');
25    ylabel('y');
26    zlabel('u');
27    colorbar;
28 end
```

```
30 function u = mg_step(u, f, h, level)
31     % Multigrid recursive V-cycle step
32     if level == 0
33         % Coarsest level: solve directly
34         u = solve_coarsest(f, h);
35     else
36         % Pre-smoothing
37         u = gauss_seidel(u, f, h, 3);
38
39         % Compute residual
40         residual = f - laplacian(u, h);
41
42         % Restrict residual to coarse grid
43         residual_coarse = restrict(residual);
44
45         % Zero initial guess for error on coarse grid
46         error_coarse = zeros(size(residual_coarse));
47
48         % Recursively solve for error
49         h_coarse = 2 * h;
50         error_coarse = mg_step(error_coarse, residual_coarse, h_coarse, level - 1);
51
52         % Prolongate error to fine grid and correct
53         error_fine = prolong(error_coarse);
54         u = u + error_fine;
55
56         % Post-smoothing
57         u = gauss_seidel(u, f, h, 3);
58     end
59 end
```


写一个多层网格法的简单示例

```
61 function u = v_cycle(u, f, h, num_cycles)
62     % Perform multigrid V-cycle
63     for cycle = 1:num_cycles
64         u = mg_step(u, f, h, log2(size(u, 1)) - 1);
65     end
66 end
67
68 function u = gauss_seidel(u, f, h, num_sweeps)
69     % Gauss-Seidel relaxation
70     n = size(u, 1);
71     for sweep = 1:num_sweeps
72         for i = 2:n-1
73             for j = 2:n-1
74                 u(i, j) = 0.25 * (h^2 * f(i, j) + u(i-1, j) + u(i+1, j) + u(i, j-1) + u(i, j+1));
75             end
76         end
77     end
78 end
79
80 function res = laplacian(u, h)
81     % Compute the discrete Laplacian of u
82     res = (circshift(u, [-1, 0]) + circshift(u, [1, 0]) + circshift(u, [0, -1]) + circshift(u, [0, 1]) - 4 * u) / h^2;
83 end
84
85 function u_coarse = restrict(u)
86     % Restriction operator (full-weighting)
87     n_coarse = (size(u, 1) - 1) / 2 + 1;
88     u_coarse = zeros(n_coarse);
89     for i = 2:n_coarse-1
90         for j = 2:n_coarse-1
91             u_coarse(i, j) = 0.25 * u(2*i-1, 2*j-1) + ...
92                 0.125 * (u(2*i, 2*j-1) + u(2*i-2, 2*j-1) + u(2*i-1, 2*j) + u(2*i-1, 2*j-2)) + ...
93                 0.0625 * (u(2*i, 2*j) + u(2*i, 2*j-2) + u(2*i-2, 2*j) + u(2*i-2, 2*j-2));
94         end
95     end
96 end
```

```
98 function u_fine = prolong(u)
99     % Prolongation operator (bilinear interpolation)
100     n_fine = 2 * (size(u, 1) - 1) + 1;
101     u_fine = zeros(n_fine);
102     for i = 1:size(u, 1)
103         for j = 1:size(u, 1)
104             u_fine(2*i-1, 2*j-1) = u(i, j);
105         end
106     end
107     for i = 1:size(u, 1)-1
108         for j = 1:size(u, 1)-1
109             u_fine(2*i, 2*j-1) = 0.5 * (u(i, j) + u(i+1, j));
110             u_fine(2*i-1, 2*j) = 0.5 * (u(i, j) + u(i, j+1));
111             u_fine(2*i, 2*j) = 0.25 * (u(i, j) + u(i+1, j) + u(i, j+1) + u(i+1, j+1));
112         end
113     end
114 end
115
116 function u = solve_coarsest(f, h)
117     % Solve on coarsest grid using direct method
118     n = size(f, 1);
119     A = gallery('poisson', n - 2) / h^2;
120     f_vec = reshape(f(2:end-1, 2:end-1), [], 1);
121     u_vec = A \ f_vec;
122     u = zeros(n);
123     u(2:end-1, 2:end-1) = reshape(u_vec, n-2, n-2);
124 end
```



Why do you still write a code like an ancient man? Why do you still write a code anyways?

Can you tell which code is better when you see it? Can you tell AI what kind of code you need?

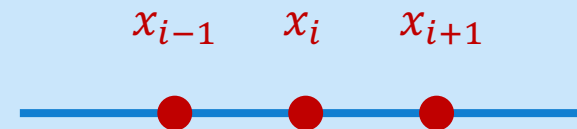
几何多层网格法的实现

无矩阵GMG实现方式:

- 存储量大幅度降低, 减少内存使用量
- 可对相似运算重排/合并, 提高cache命中率
- 可对部分模块进行细粒度并行优化

提高GMG实现的通用性:

- 基于稀疏矩阵运算进行, 通用性强
- 与代数多层网格法 (AMG) 的结构相同
- 利用稀疏矩阵运算库 (如SpMV内核)



$$A[i, :] u = -1 * u_{i-1} + 2 * u_i - 1 * u_{i+1}$$

Fixed stencil computation

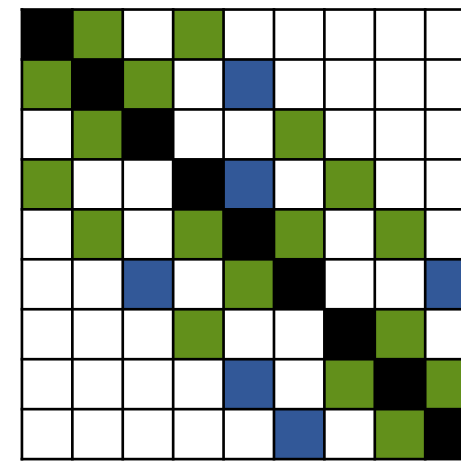
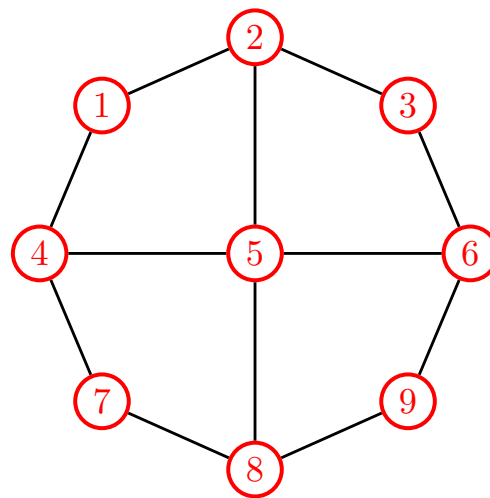
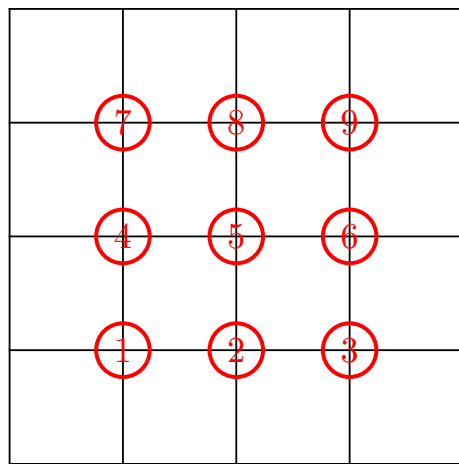
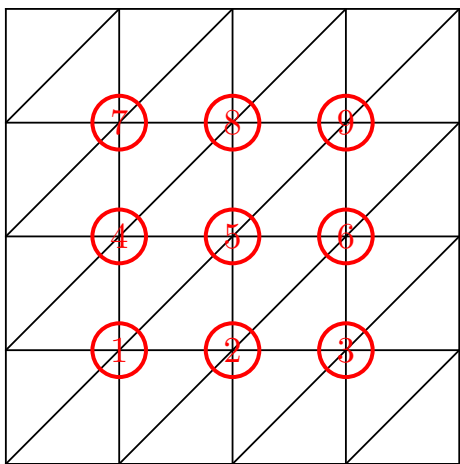
$$u = u + \omega D^{-1} (f - Au)$$

$$u = u + P(RAP)^{-1} R(f - Au)$$

从GMG到AMG

GMG在实际应用中的困难:

- 网格限制多: 效率依赖于结构化嵌套加密网格的信息, 实际应用中网格往往无法满足要求
- 通用性不高: 程序是问题相关的 (白盒子), 需要case-by-case地设计方法
- 应用难度大: 很难应用在有各种限制条件的实际问题中



- 系数矩阵可以对应一个图 (带权或者不带权), 对称问题 → 无向图, 非对称问题 → 有向图
- 可根据临接图反推方程或离散方法的部分信息, 构造operator-dependent方法 → 代数多层网格法

经典代数多重网格法C-AMG

Strong n-coupling: $-a_{i,j} \geq \theta_{\text{str}} |\min_k a_{i,k}|$

- $A = (a_{i,j}) \in \mathbb{R}^{N \times N}$ is an M-matrix
- $G = (V, E)$ is the corresponding graph of A
- $S_i := \{j \in N_i : j \text{ strongly coupled to } i\}$
- $S_i^T := \{j \in V : i \in S_j\}$, set affected by i

```
1 U ← V, C ← ∅, F ← ∅;
2 while U ≠ ∅
3     λi ← 2|SiT ∩ F| + |SiT ∩ U|, i ∈ U;
4     k ← arg max{λi, i ∈ U};
5     C ← C ∪ {k}, U ← U \ {k};
6     F ← F ∪ SkT, U ← U \ SkT;
7 end
```

$$A = \begin{pmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{pmatrix} \quad P := \begin{pmatrix} W \\ I \end{pmatrix}$$

$$a_{ii}e_i + \sum_{j \in N_i} a_{ij}e_j = 0, \quad i \in F.$$

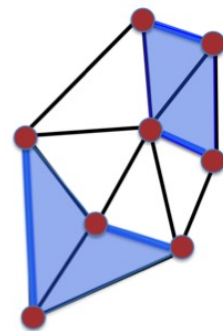
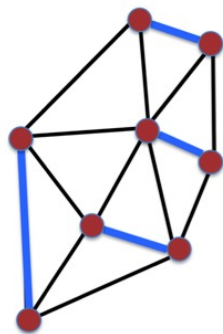
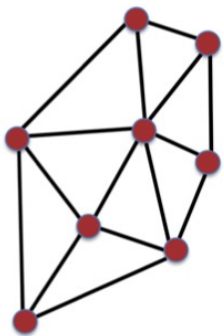
$$a_{ii}e_i + \alpha_i \sum_{j \in N_i \cap C} a_{ij}e_j = 0,$$

$$\text{where } \alpha_i := \frac{\sum_{k \in N_i} a_{ik}}{\sum_{k \in N_i \cap C} a_{ik}}$$

$$W = \text{diag}(A_{fc}\mathbf{1}_c)^{-1}A_{fc}.$$

Direct Interpolation

聚集代数多重网格法A-AMG



- Tentative prolongation

$$P_{ij} := \begin{cases} 1, & i \in \mathcal{A}_j \\ 0, & i \notin \mathcal{A}_j \end{cases}$$

$$P := \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{pmatrix},$$

$$R := P^T = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix}$$

- Coarser problem matrix

$$A_c := RAP = P^T AP$$

- 算法的复杂度低, 但收敛性受到影响

- 利用光滑聚集方法SA-AMG
- 利用更精确的CGC方法: W-cycle, AMLI-cycle, Krylov-cycle

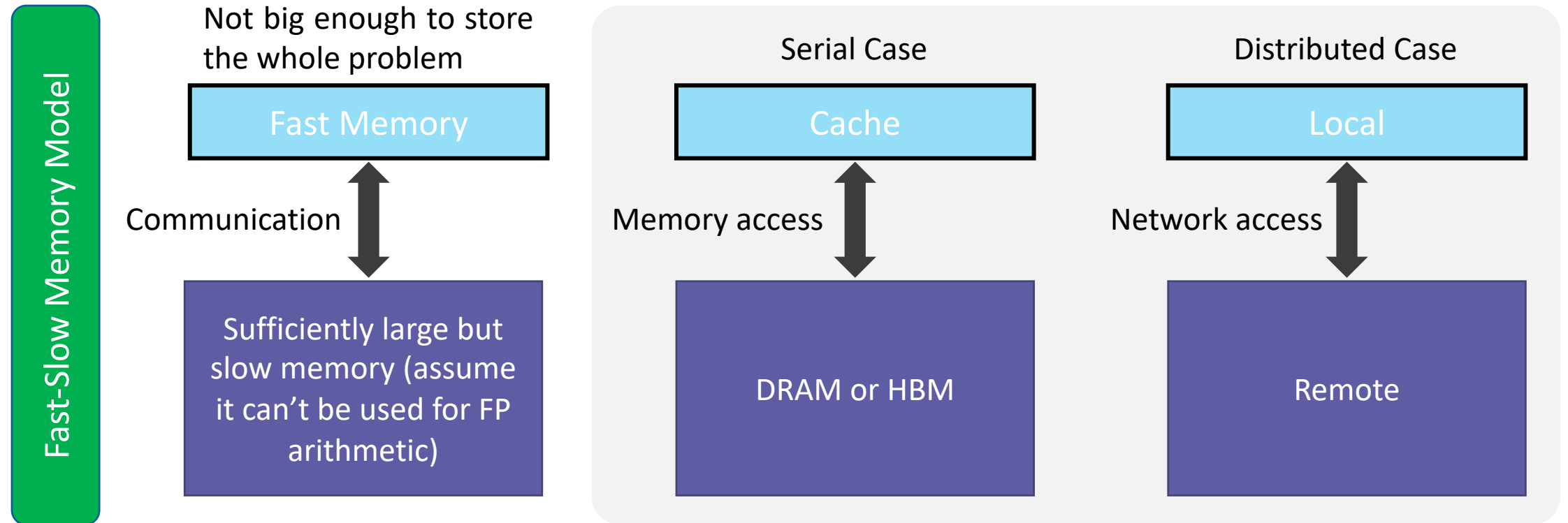
数值模拟的重要内核：快速Poisson解法器

问题规模	网格剖分	64 ³			128 ³	256 ³	512 ³	1024 ³
	变量个数	0.25M			2M	16M	135M	1024M
稀疏直接法 @北京超算	计算核数	8x1	16x1	32x1	16x8	16x64	16x512	16x1024
	求解时间	5.38s	3.86s	3.26s	59.78s	999.46s	/	/
GMG@CPU	求解时间	0.030s			0.303s	2.815s	23.54s	/
GMG@GPU	求解时间	0.013s			0.026s	0.045s	0.097s	0.715s

三维Poisson方程（均匀网格七点差分格式）的线性解法器对比，稀疏直接法软件Intel MKL Pardiso（北京超级云超算）和几何多重网格法FASP（笔记本电脑、nVidia A100）：线程数x进程数。2020年，北京超级云计算中心A分区以Linpack测试性能3.74PFlops，获中国HPC TOP100榜单第三名及通用CPU算力第一名。单节点配两颗32核AMD EPYC7452，256GB内存。

考虑通信开销的性能模型

$$\text{Communication Time} = \text{Latency} + \text{Num of Bytes Moved} \div \text{Bandwidth}$$



Ref: CS267 lecture notes on J. Demmel's webpage: <https://people.eecs.berkeley.edu/~demmel/>

常用AMG迭代法软件包

支持共享内存与分布式并行及GPU的C语言库，由美国LLNL研发，最早于2000.1.14开源发布，最新版是2.30.0

HYPRE

支持共享内存与分布式并行的F90库，最早于2008.2发布，于2012.1 (3.0版)对聚集算法进行大改，最新版是4.2.2

AGMG

支持共享内存并行及GPU/DCU的C语言库，最早于2010.4.1公开发布0.1.0，最新版是2.8.7

FASP

支持共享内存与分布式并行及GPU的C++库，PETSc中的预条件子，由Mark Adams等研发，2012.6.5出现在PETSc 3.3中

GAMG

支持共享内存与分布式并行及GPU的C++库，Sandia实验室Trilinos项目的一部分，最早于2014.10发布（出现在11.12版中）

MueLu

由国防科技大学研发的并行代数多重网格算法库，支持分布式和共享式的C++库，最早于2018年启动，目前最新版是1.0

YHAMG

PyAMG

Python库，由Nathan Bel、Luke Olson、Jacob Schroder和Ben Southworth开发，始于2008年，于2013.7.10提交了2.1版到GitHub，最新版是5.0.1

JXPAMG

支持共享与分布式的C库，由北京九所与湘潭大学联合研发，项目于2009年开始启动，最新版是2.0

CUSP

支持GPU的头文件库，由Steven Dalton、Nathan Bell等开发，项目于2010.7.10发布0.1.0版，最新版是2015发布的0.5.1版

AmgX

支持分布式并行及GPU，由NVIDIA开发，最早于2014.5.15发布版本1.0，最新版是2.4.0

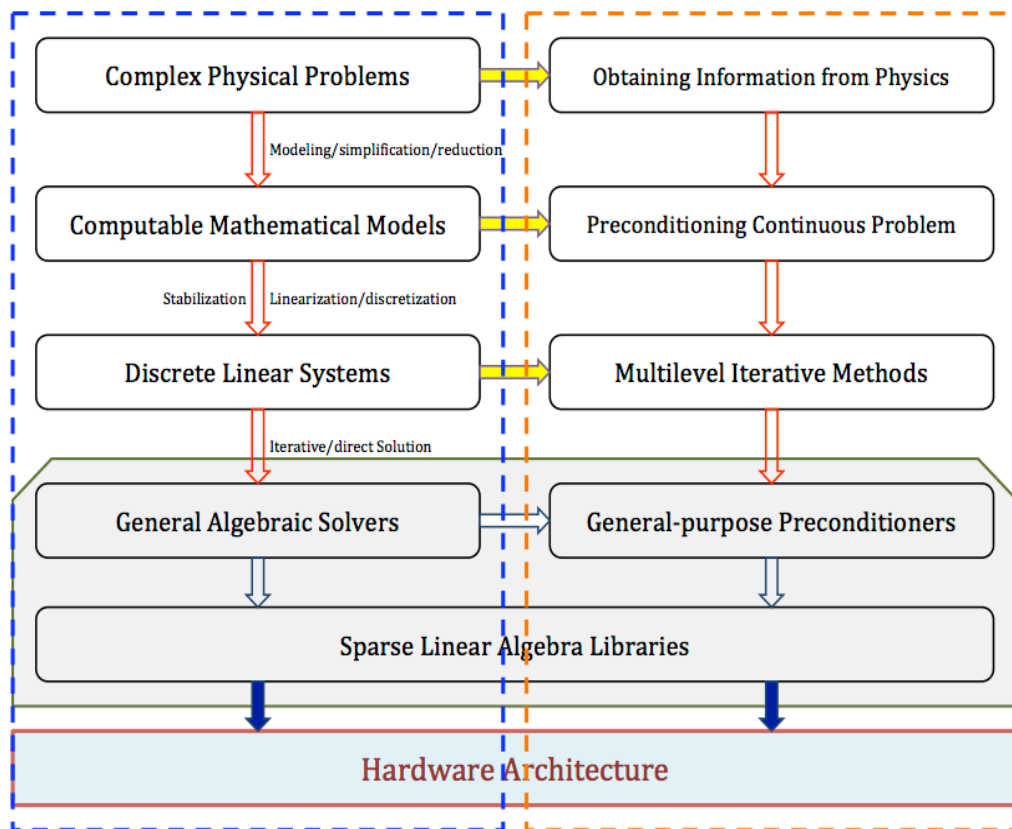
AMGCL

支持共享与分布式并行的C++头文件，由俄罗斯科学院的Denis Demidov研发，于2017.5.3提交了0.9.0版到GitHub，最新版是1.4.4

开源解法器FASP项目

FASP 开源项目网址

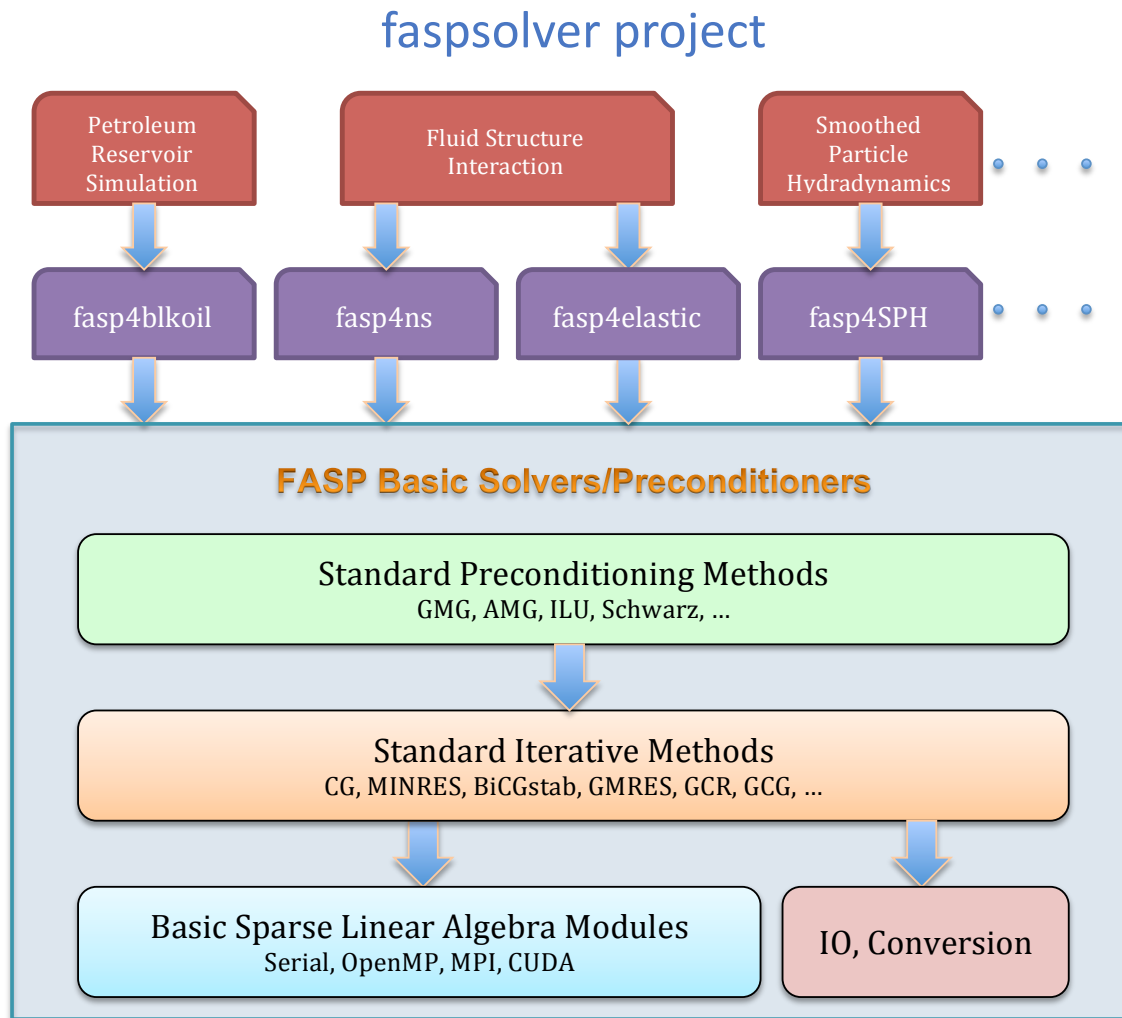
<http://www.multigrid.org/fasp>
<https://github.com/FaspDevTeam/faspsolver>
<https://gitee.com/faspdevteam/faspxx>



FASP及相关开源软件项目：

- faspsolver, 开源迭代解法器项目
- fasp4ns, 开源流体解法器项目
- fasp4cuda, 开源GPU解法器项目
- fasp4dcu, 开源国产GPU解法器项目
- fasp4blkoil, 开源油藏模拟解法器项目
- faspxx, 开源并行迭代解法器项目
- StructMG, 拓扑结构化网格求解器项目
- SemiStructMG, 半结构化网格求解器项目

fasp solver 解法器软件简介



Fast Auxiliary Space Preconditioning (FASP) Solver Library: README

Introduction

The FASP package is designed for developing and testing new efficient solvers and preconditioners for discrete partial differential equations (PDEs) or systems of PDEs. The main components of the package are standard Krylov methods, algebraic multigrid methods, and incomplete factorization methods. Based on these standard techniques, we build efficient solvers, based on the framework of Auxiliary Space Preconditioning, for several complicated applications. Current examples include the fluid dynamics, underground water simulation, the black oil model in reservoir simulation, and so on.

Install

To compile, you need a C99 compiler (and a F90 compiler if you need Fortran examples). By default, we use GNU gcc/gfortan, respectively.

Configuring and building the FASP library and test suite requires CMake 2.8 or higher <http://www.cmake.org/>.

The command to configure is:

```
$ mkdir Build; cd Build; cmake ..
```

After successfully configuring the environment, just run:

```
$ make // to compile the FASP static library
```

To install the FASP library and executables, run:

```
$ make install
```

faspsolver安装选项介绍



```

FASPSOLVER
├── .vscode
├── base
├── benchmark
├── build
├── data
├── doc
├── include
├── lib
├── log
├── modules
├── test
├── tutorial
├── util
├── vs19
├── xcode
├── .gitignore
├── CMakeLists.txt
├── Config.mk
├── FASP_GUI_help.txt
├── FASP_install.tcl
├── FASP.mk
├── FASP.mk.example
├── FASP.mk.umfpack
├── INSTALL
├── License
└── README.md

```

```

CMakeLists.txt
1 # CMakeLists for faspsolver
2 #
3 # Author          Date          Action
4 # -----
5 # Ludmil Zikatanov Aug/08/2015  Create CMakeLists
6 # Chensong Zhang   Oct/20/2017  Update to new FASP code
7 # Ludmil Zikatanov Aug/08/2019  Fix installation problem for cmake 3.14+
8 # Chensong Zhang   Mar/13/2021  Replace FASP_SOURCE_DIR with general dir
9 # Chensong Zhang   Mar/23/2021  Add headers and backup target
10 # Chensong Zhang   May/10/2021  Test the new OpenMP code
11 #
12 # Some sample usages (It is better to use a separate dir for building):
13 #   mkdir Build; cd Build; cmake ..           // build in Release configuration
14 #   cmake -DCMAKE_BUILD_TYPE=Debug ..        // build in Debug configuration
15 #   cmake CC=clang ..                          // build with specified compiler
16 #   cmake -DCMAKE_VERBOSE_MAKEFILE=ON ..      // build with verbose on
17 #   cmake -DUSE_UMFPACK=ON ..                  // build with UMFPACK package support
18 #   cmake -DOPENMP=ON ..                       // build with OpenMP support
19 #
20 #####
21 ## General environment setting
22 #####
23
24 # Minimum cmake version needed
25 cmake_minimum_required (VERSION 2.8.12)
26
27 # Helper modules
28 include(CheckFunctionExists)
29 include(CheckIncludeFile)
30
31 set(GDB          1 CACHE BOOL "debugging or not")
32 set(OPENMP       0 CACHE BOOL "Openmp use")
33 set(USE_MUMPS    0 CACHE BOOL "MUMPS use")
34 set(USE_UMFPACK  0 CACHE BOOL "UMFPACK use")
35 set(USE_SUPERLU  0 CACHE BOOL "SUPERLU use")
36 set(USE_PARDISO  0 CACHE BOOL "PARDISO use")
37 set(USE_DOXYGEN  0 CACHE BOOL "Doxygen use")

```

fasp solver 简单算例 (C语言)



```
1  /*! \file poisson-pcg.c
2  *
3  * \brief The third test example for FASP: using PCG to solve
4  *       the discrete Poisson equation from P1 finite element.
5  *       C version.
6  *
7  * \note Solving the Poisson equation (P1 FEM) with PCG: C version
8  *
9  *-----
10 * Copyright (C) 2012--Present by the FASP team. All rights reserved.
11 * Released under the terms of the GNU Lesser General Public License 3.0 or later.
12 *-----
13 */
14
15 #include "fasp.h"
16 #include "fasp_functs.h"
17
18 /**
19 * \fn int main (int argc, const char * argv[])
20 *
21 * \brief This is the main function for the third example.
22 *
23 * \author Feiteng Huang
24 * \date 05/17/2012
25 *
26 * Modified by Chensong Zhang on 09/22/2012
27 * Modified by Chensong Zhang on 12/23/2018: Fix memory leakage
28 */
29 int main (int argc, const char * argv[])
30 {
31     input_param    inparam; // parameters from input files
32     ITS_param      itparam; // parameters for itsolver
33     AMG_param      amgparam; // parameters for AMG
34     ILU_param      iluparam; // parameters for ILU
35
36     printf("\n=====");
37     printf("\n|| FASP: PCG example -- C version ||");
38     printf("\n=====\\n\\n");
39
40     // Step 0. Set parameters: We can use ini/pcg.dat
41     fasp_param_set(argc, argv, &inparam);
42     fasp_param_init(&inparam, &itparam, &amgparam, &iluparam, NULL);
43
44     // Set local parameters
45     const SHORT print_level = itparam.print_level;
46     const SHORT pc_type     = itparam.precond_type;
47     const SHORT stop_type   = itparam.stop_type;
48     const INT   maxit       = itparam.maxit;
49     const REAL  tol         = itparam.tol;
50
```

```
51 // Step 1. Get stiffness matrix and right-hand side
52 // Read A and b -- P1 FE discretization for Poisson. The location
53 // of the data files is given in "ini/pcg.dat".
54 dCSRmat A;
55 dvector b, x;
56 char filename1[512], *datafile1;
57 char filename2[512], *datafile2;
58
59 // Read the stiffness matrix from matFE.dat
60 memcpy(filename1, inparam.workdir, STRLEN);
61 datafile1="csrmat_FE.dat"; strcat(filename1, datafile1);
62
63 // Read the RHS from rhsFE.dat
64 memcpy(filename2, inparam.workdir, STRLEN);
65 datafile2="rhs_FE.dat"; strcat(filename2, datafile2);
66
67 fasp_dcsrvec_read2(filename1, filename2, &A, &b);
68
69 // Step 2. Print problem size and PCG parameters
70 if (print_level>PRINT_NONE) {
71     printf("A: m = %d, n = %d, nnz = %d\\n", A.row, A.col, A.nnz);
72     printf("b: n = %d\\n", b.row);
73     fasp_param_solver_print(&itparam);
74 }
75
76 // Step 3. Setup preconditioner
77 // Preconditioner type is determined by pc_type
78 precond *pc = fasp_precond_setup(pc_type, &amgparam, &iluparam, &A);
79
80 // Step 4. Solve the system with PCG as an iterative solver
81 // Set the initial guess to be zero and then solve it using PCG solver
82 // Note that we call PCG interface directly. There is another way which
83 // calls the abstract iterative method interface; see poisson-its.c for
84 // more details.
85 fasp_dvec_alloc(A.row, &x);
86 fasp_dvec_set(A.row, &x, 0.0);
87
88 fasp_solver_dcsr_pcg(&A, &b, &x, pc, tol, maxit, stop_type, print_level);
89
90 // Step 5. Clean up memory
91 // First clean up the AMG data if you are using AMG as preconditioner
92 fasp_amg_data_free(((precond_data *)pc->data)->mg1_data, &amgparam);
93
94 // Clean up the pcd data
95 if (pc_type!=PREC_NULL) fasp_mem_free(pc->data);
96 fasp_mem_free(pc);
97
98 // Clean up coefficient matrix, right-hand side, and solution
99 fasp_dcsr_free(&A);
100 fasp_dvec_free(&b);
101 fasp_dvec_free(&x);
102
103 return FASP_SUCCESS;
104 }
```

fasp solver 简单算例 (Fortran 语言)



```
1  !> \file poisson-pcg.f90
2  !>
3  !> \brief The third test example for FASP: using PCG to solve
4  !>       the discrete Poisson equation from P1 finite element.
5  !>       F90 version.
6  !>
7  !> \note Solving the Poisson equation (P1 FEM) with PCG: F90 version
8  !>
9  !> -----
10 !> Copyright (C) 2012--Present by the FASP team. All rights reserved.
11 !> Released under the terms of the GNU Lesser General Public License 3.0 or later.
12 !> -----
13
14 program test
15
16     implicit none
17
18     double precision, dimension(:), allocatable :: u,b
19     double precision, dimension(:), allocatable :: a
20     integer,          dimension(:), allocatable :: ia,ja
21
22     integer          :: iufile, n, nnz, i, prt_lvl, maxit
23     double precision :: tol
24
25     print*, ""
26     write(*,"(A)") "=====
27     write(*,"(A)") "||  FASP: PCG example -- F90 version  ||"
28     write(*,"(A)") "=====
29     print*, ""
30
31     ! Step 0: user defined variables
32     prt_lvl = 3
33     maxit = 500
34     tol = 1.0d-6
35     iufile = 1
36
37     ! Step 1: read A and b
38
39     !==> Read data A from file
40     open(unit=iufile,file='../data/csrmat_FE.dat')
```

```
41
42     read(iufile,*) n
43     allocate(ia(1:n+1))
44     read(iufile,*) (ia(i),i=1,n+1)
45
46     nnz=ia(n+1)-ia(1)
47     allocate(ja(1:nnz),a(1:nnz))
48     read(iufile,*) (ja(i),i=1,nnz)
49     read(iufile,*) (a(i),i=1,nnz)
50
51     close(iufile)
52
53     !==> Read data b from file
54     open(unit=iufile,file='../data/rhs_FE.dat')
55
56     read(iufile,*) n
57     allocate(b(1:n))
58     read(iufile,*) (b(i),i=1,n)
59
60     close(iufile)
61
62     !==> Shift the index to start from 0 (for C routines)
63     forall (i=1:n+1) ia(i)=ia(i)-1
64     forall (i=1:nnz) ja(i)=ja(i)-1
65
66     ! Step 2: Solve the system
67
68     !==> Initial guess
69     allocate(u(1:n))
70     u=0.0d0
71     call fasp_fwapper_dcsr_krylov_amg(n,nnz,ia,ja,a,b,u,tol,maxit,prt_lvl);
72
73     ! Step 3: Clean up memory
74     deallocate(ia,ja,a)
75     deallocate(b,u)
76
77 end program test
78
```

fasp solver 算法参数配置



```

10 %-----%
11 % parameters for multilevel iteration %
12 %-----%
13
14 AMG_type = C % C classic AMG
15 % SA smoothed aggregation
16 % UA unsmoothed aggregation
17 AMG_cycle_type = V % V V-cycle | W W-cycle
18 % A AMLI-cycle | NA Nonlinear AMLI-cycleA
19 AMG_tol = 1e-8 % tolerance for AMG
20 AMG_maxit = 100 % number of AMG iterations
21 AMG_levels = 20 % max number of levels
22 AMG_coarse_dof = 500 % max number of coarse degrees of freedom
23 AMG_coarse_scaling = OFF % switch of scaling of the coarse grid correction
24 AMG_amli_degree = 2 % degree of the polynomial used by AMLI cycle
25 AMG_nl_amli_krylov_type = 6 % Krylov method in NLAMLI cycle: 6 FGMRES | 7 GCC
26
27 %-----%
28 % parameters for AMG smoothing %
29 %-----%
30
31 AMG_smoother = GS % GS | JACOBI | SGS
32 % SOR | SSOR | GSOR | SGSOR | POLY
33 AMG_ILU_levels = 0 % number of levels using ILU smoother
34 AMG_SWZ_levels = 0 % number of levels using Schwarz smoother
35 AMG_relaxation = 1.1 % relaxation parameter for SOR smoother
36 AMG_polynomial_degree = 3 % degree of the polynomial smoother
37 AMG_presmooth_iter = 2 % number of presmoothing sweeps
38 AMG_postsmooth_iter = 2 % number of postsmoothing sweeps
39
40 %-----%
41 % parameters for classical AMG SETUP %
42 %-----%
43
44 AMG_coarsening_type = 1 % 1 Modified RS
45 % 3 Compatible Relaxation
46 % 4 Aggressive
47 AMG_interpolation_type = 1 % 1 Direct | 2 Standard | 3 Energy-min
48 AMG_strong_threshold = 0.6 % Strong threshold
49 AMG_truncation_threshold = 0.4 % Truncation threshold
50 AMG_max_row_sum = 0.9 % Max row sum

```

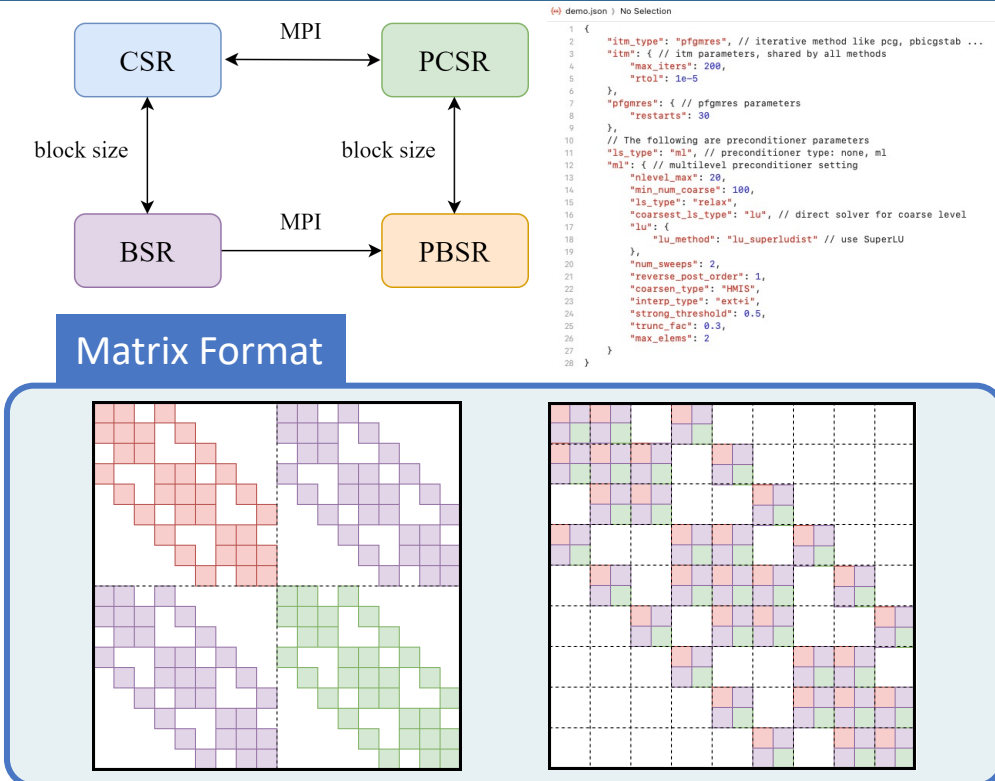
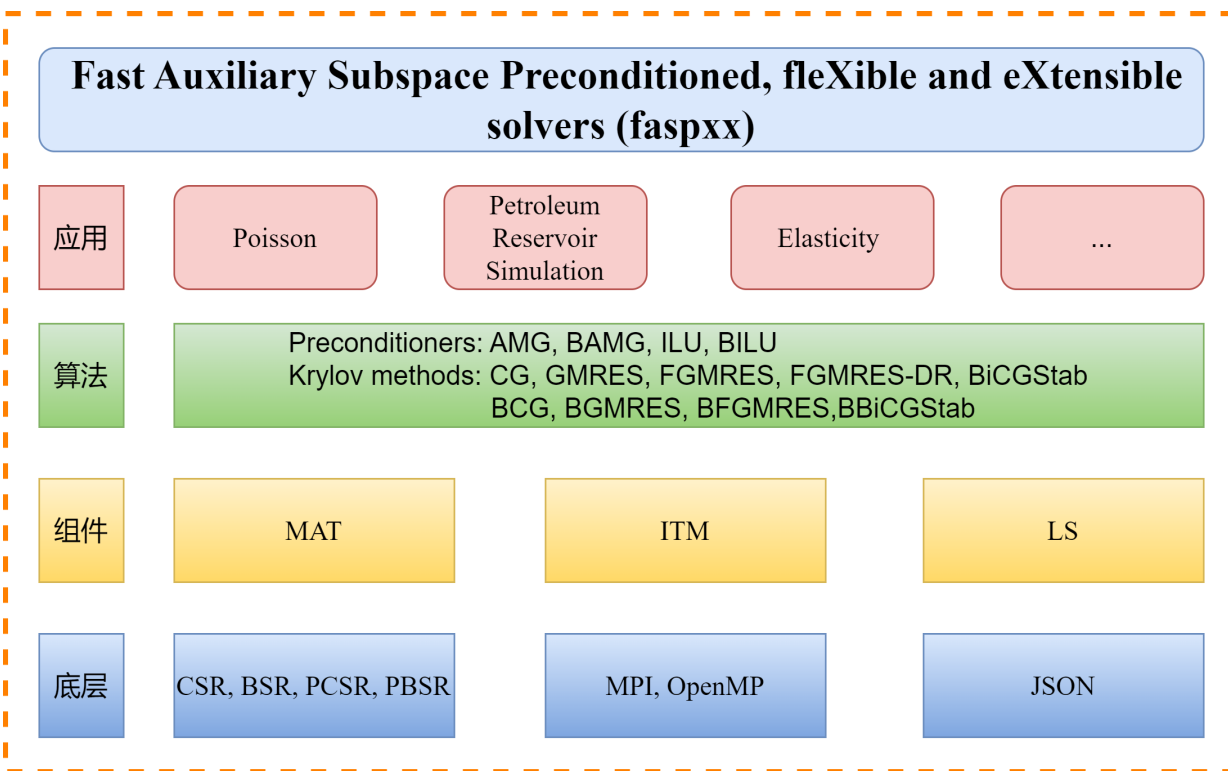
Problem	DOF	RS-V-CG	UA-NA-CG	hypre	AGMG
2D 5pt	1M	1.79	1.43	1.96	1.73
2D 5pt	4M	8.71	6.04	8.45	6.61
2D 9pt	1M	1.82	2.07	2.25	2.24
2D 9pt	4M	7.63	8.39	8.88	9.42
3D 7pt	$\frac{1}{4}$ M	1.05	0.37	1.83	0.43
3D 7pt	2M	10.86	3.28	19.04	3.71
3D 27pt	$\frac{1}{4}$ M	2.09	0.94	3.26	1.79
3D 27pt	2M	20.0	8.53	34.54	20.29

Test Device: Intel Core i5 2.6GHz, 8GB RAM, gcc 4.9.2 -O2. Software ver: FASP 1.7.0, hypre 2.10.0b, AGMG 3.2.0 (default parameters). Computing time (seconds) of the AMG-preconditioned CG method. We solve the 2D/3D Poisson equation with one processing core. Stopping criteria: relative residual is less than 1E-6.

faspvx并行解法器软件简介



- A flexible and extensible package of iterative solvers/preconditioners: <https://gitee.com/faspdevteam/faspvx>
- Features: Parallel (MPI/OpenMP) support; a unified design for solver/precond/smoothing design, KSM: CG, BiCGStab, GMRES(m), FGMRES-DR, ...; controls via a JSON file



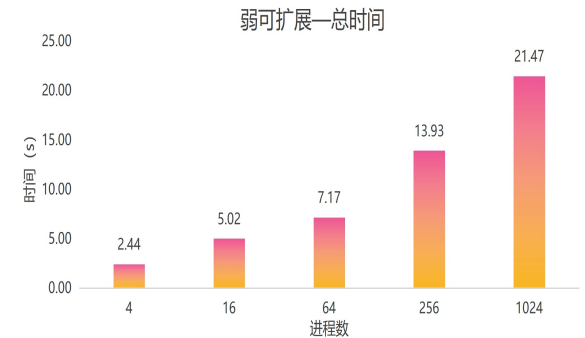
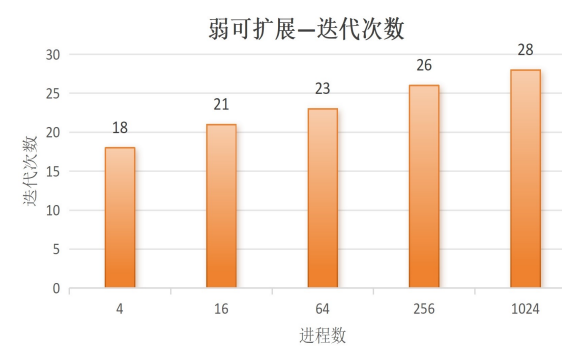
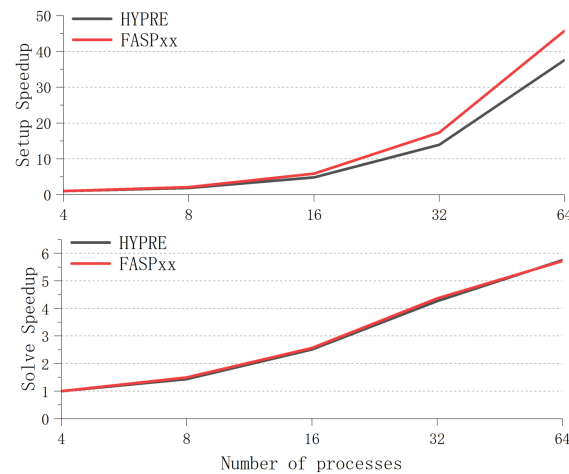
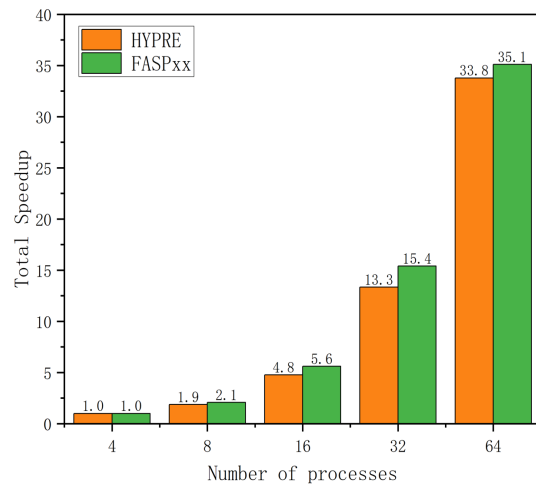
faspxx的并行性能测试 (C-AMG解法器)

Test 1. FEM for Poisson, grid: 2048x2048, dof: 4M, AMG-CG

BoomerAMG (default, OC=2.24)					FASPxx CAMG (OC=1.88)				
NP	IT	Setup (s)	Solve (s)	Total (s)	IT	Setup (s)	Solve (s)	Total (s)	
4	14	313.97	6.48	320.44	18	180.09	8.16	188.25	
8	15	166.90	4.50	171.41	18	85.45	5.43	90.88	
16	15	64.76	2.58	67.34	18	30.43	3.18	33.60	
32	15	22.50	1.52	24.02	18	10.36	1.87	12.23	
64	15	8.36	1.13	9.48	18	3.93	1.43	5.36	

Test 2. FEM for Poisson, dof/np: 64,000, AMG-CG

FASPxx CAMG (OC=1.72)					
NP	Mesh	IT	Setup (s)	Solve (s)	Total (s)
4	512x512	18	2.00	0.43	2.44
16	1024x1024	21	4.35	0.67	5.02
64	2048x2048	23	5.79	1.38	7.17
256	4096x4096	26	7.58	6.36	13.93
1024	8192x8192	28	10.29	11.18	21.47



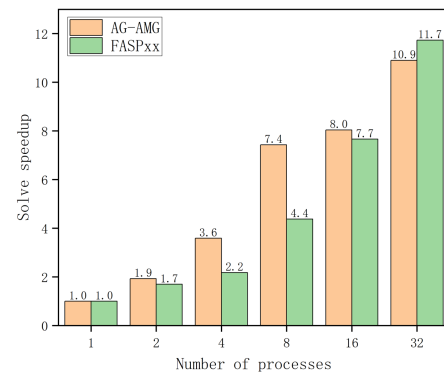
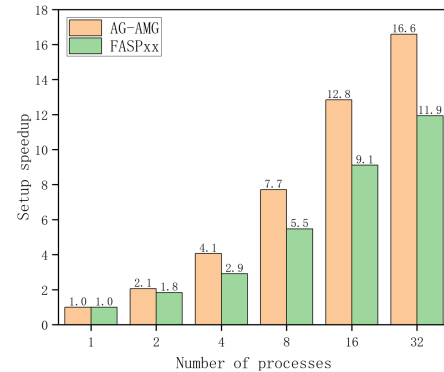
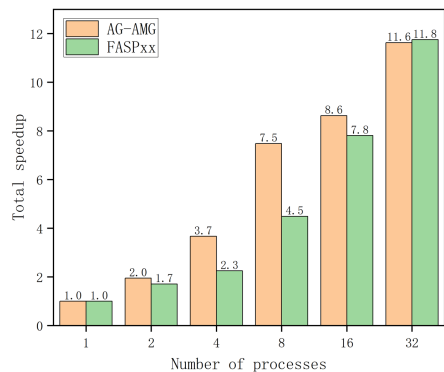
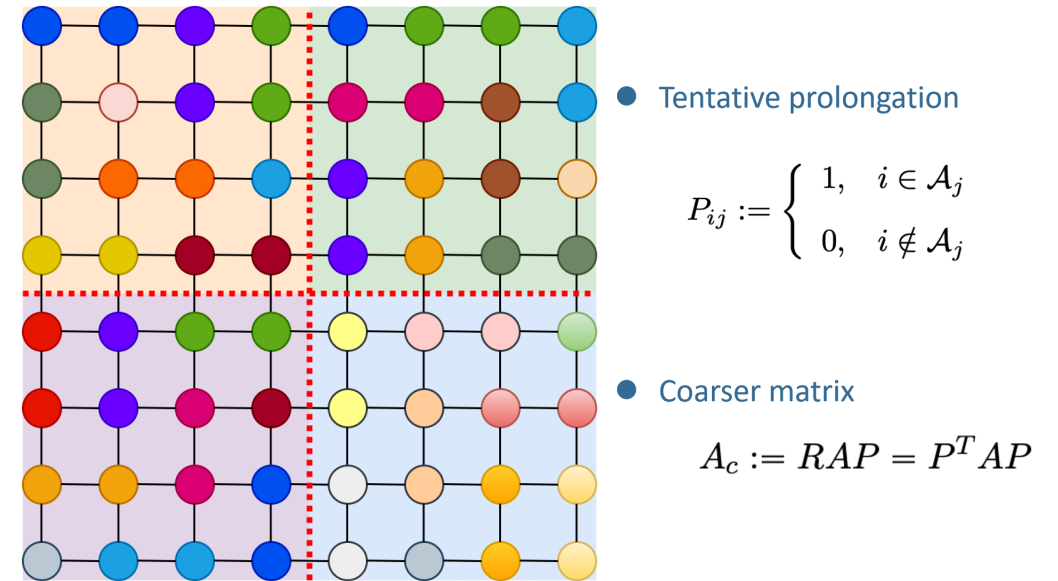
Strong and weak scalability performance test for the discrete Poisson's equation (finite element)

faspxx的并行性能测试 (A-AMG解法器)

Test 3. FDM for Poisson, grid: 4096x4096, dof: 16M, AMG-CG

NP	AG-AMG (OC=1.14)				FASPxx UA-AMG (OC=1.14)			
	IT	Setup (s)	Solve (s)	Total (s)	IT	Setup (s)	Solve (s)	Total (s)
1	50	5.69	25.50	31.19	48	4.63	33.27	37.90
2	50	2.76	13.20	15.96	51	2.52	19.58	22.10
4	50	1.40	7.10	8.50	82	1.59	15.27	16.86
8	50	0.74	3.43	4.17	80	0.85	7.60	8.45
16	82	0.44	3.17	3.61	80	0.51	4.34	4.85
32	85	0.34	2.34	2.68	80	0.39	2.84	3.22

Parallel Pairwise aggregation method



For the discrete Poisson's equation (finite difference), strong scalability performance of the faspxx solver is similar to that of AMG

线性解法器不可能三角

Q: 如何改进Multigrid方法实现? 目标? 计算资源? 用户类型? 开发代价? 有无高效算法?

高效性

Efficient, optimal, and scalable

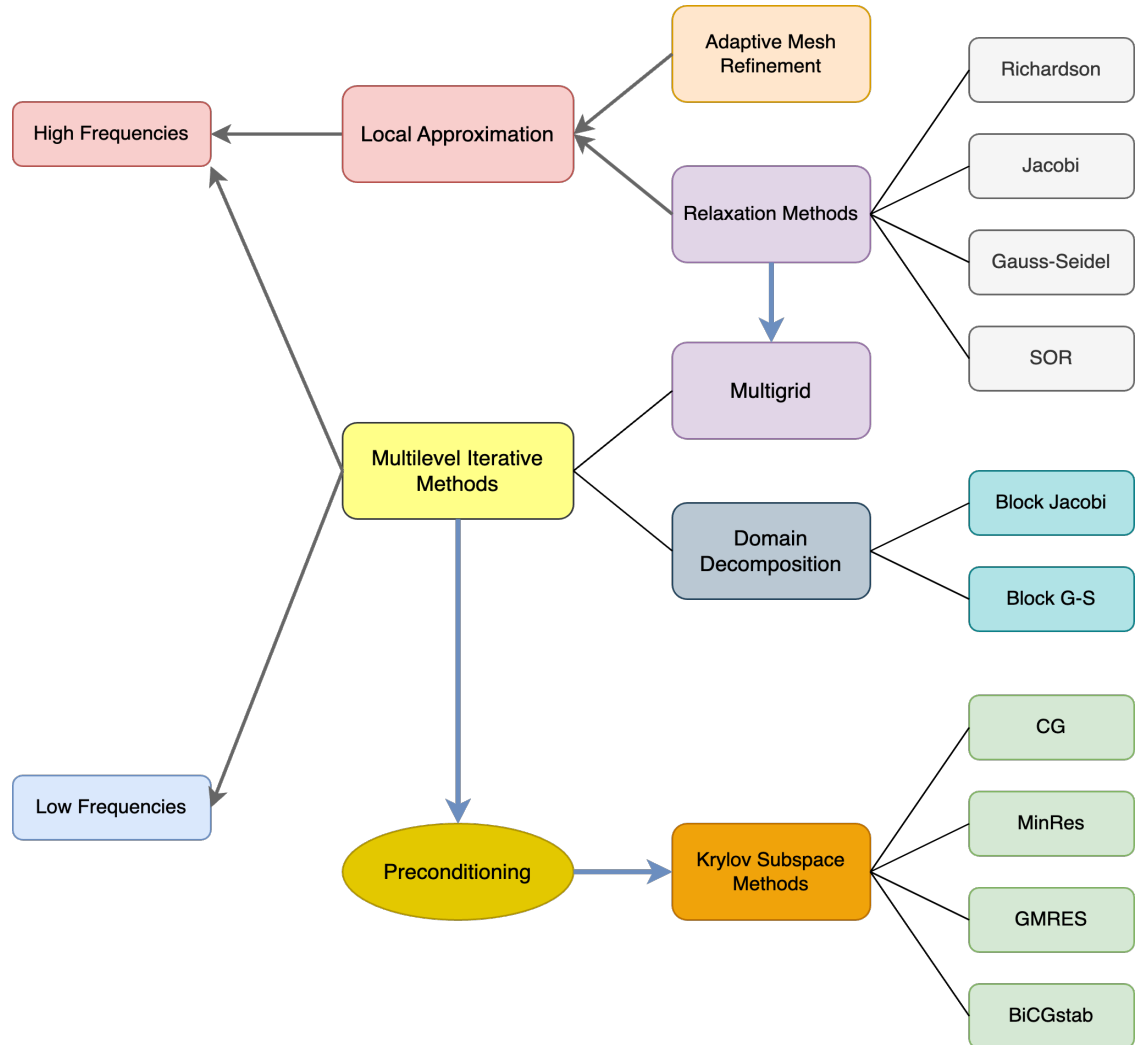
稳健性

Robust, resilient, and reliable

易用性

Applicable, user-friendly, and portable

如何选择求解方法



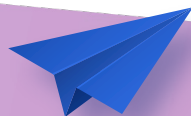
- Achi Brandt: *“The optimal method might not be the fastest”*
- Standard Krylov subspace methods work fine, but don't count on them
- Matrix-free implementation is preferred when applicable
- Iain Duff: *“Real men use direct methods”*
- Use direct methods whenever possible (only for moderate-size problems)
- **Think about your solution method as early as possible for your simulation**

端到端时间可分为如下3部分:

1. 分析
2. 准备
3. 求解

矩阵和向量的读入、格式转换、分发至多进程、矩阵坐标排序不列入统计时间。

直接法和迭代法对于上述3步的定义略有不同。



中国科学院大学
夏季强化课程
2022

Fast Solvers for
Large Algebraic Systems

Brief Introduction on This Course

快速解法器课程

做解法器预处理, 包括图分析、图优化、
iso的phase=11 (注意, pardiso phase=11
。 pardiso phase=22。
pardiso phase=33。

竞赛说明

赛题名称	solverchallenge23_01
阶数非零元数	2,097,152
非零元数	14,581,760
应用领域	激光聚变
来源与背景描述	PDE: 辐射流体力学二维数值方程
MD5	
约束	
矩阵说明	

赛题简介

竞赛方案与规则

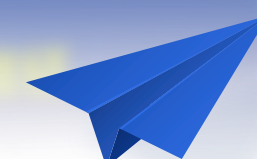
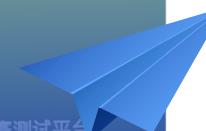
竞赛方案

竞赛组委会提供10套来源于不同应用领域的线性系统 (每套线性系统包括矩阵A和右端向量b、存储格式的描述、求解约束条件等), 参赛选手针对这10套系统进行求解, 不限制求解方法 (即迭代法、直接法或混合方法均可), 也不限制解法器软件包的来源。竞赛网站将提供程序中输入、输出与计时部分, 并开放接口供参赛选手提交自己的执行代码 (若是闭源的, 则提交链接文件)。最终将使用不同的右端向量b测试, 其求解效果 (速度、精度、浮点运算次数等) 将作为本竞赛奖项评判标准。

竞赛规则

硬件环境: 竞赛指定硬件环境, 参赛选手使用竞赛测试平台, 但使用时间将被限制, 在使用时间内参赛选手可以配置环境与测试程序, 在竞赛提供的平台

竞赛方案与规则





THANKS

Chensong Zhang, AMSS
<http://lsec.cc.ac.cn/~zhangcs>

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