Development of A Platform for Large-scale Reservoir Simulations on Parallel computers

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Abstract

This paper presents our work on designing a platform for large-scale reservoir simulations. Detailed components, such as grid and linear solver, and data structures are introduced, which can serve as a guide to parallel reservoir simulations and other parallel applications. The main objective of platform is to support implementation of various parallel reservoir simulators on distributed-memory parallel systems, where MPI (Message Passing Interface) is employed for communications among computation nodes. It provides structured grid due to its simplicity and cell-centered data is applied for each cell. The platform has a distributed matrix and vector module and a map module. The matrix and vector module is the base of our parallel linear systems. The map connects grid and linear system modules, which defines various mappings between grid and linear systems. Commonly-used Krylov subspace linear solvers are implemented, including the restarted GMRES method and the BiCGSTAB method. It also has an interface to a parallel algebraic multigrid solver, BoomerAMG from HYPRE. Parallel general-purpose preconditioners and special preconditioners for reservoir simulations are also developed. Various data structures are designed, such as grid, cell, data, linear solver and preconditioner, and some key default parameters are presented in this paper. The numerical experiments show that our platform has excellent scalability and it can simulate giant reservoir models with hundreds of millions of grid cells using thousands of CPU cores.

Keywords: platform, reservoir simulation, parallel computing, algorithm, data structure

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1. Introduction

Nowadays, various operation processes have been developed to enhance oil recovery by the oil and gas industry. Their numerical simulations are becoming more and more complicated. In the meantime, geological models from reservoirs are more and more complex, and they are also heterogeneous. Models with millions of grid cells are usually employed to obtain high resolution results. Numerical simulations may take days or even longer to complete one run using regular workstations. The long simulation time could be a problem to reservoir engineers, since dozens of simulations may be required to find optimal operations. Fast computational methods and reservoir simulators should be investigated.

Reservoir simulations have been studied for decades and various models and methods have been developed by researchers, including black oil model, compositional model, thermal model and related topics. Kaarstad et al. [6] studied oil-water model and they implemented a reservoir simulator that could solve problems with up to one million grid cells. Rutledge et al. [4] developed a compositional simulator for massive SIMD computers, which employed the IMPES (implicit pressure-explicit saturation) method. Killough et al. [3] implemented a compositional simulator for distributed-memory parallel systems. Killough et al. also used the locally refined grids in their parallel simulator to improve accuracy [7]. Dogru and his group [8, 9] developed a parallel simulator, which was capable of simulating reservoir models with one billion grid cells. Zhang et al. developed a platform for adaptive finite element and adaptive finite volume methods, which has been applied to CFD, Maxwell equation, material, electronic structures, biology and reservoir simulations [10, 11, 39], and a black oil simulator using discontinuous Galerkin method has been reported [39]. For many reservoir simulations, especially black oil simulation, most of the simulation time is spent on the solution of linear systems and it is well-known that the key of accelerating linear solvers is to develop efficient preconditioners. Many preconditioner methods have been applied to reservoir simulations, including point-wise and block-wise incomplete factorization (ILU) methods for general linear systems [13], domain decomposition methods [22], constrained pressure residual (CPR) methods for the black oil model, compositional model and extended black oil models [14, 15], multi-stage methods [17], multiple level preconditioners [38] and fast auxiliary space preconditioners (FASP) [18].

This paper presents our work on developing a parallel platform for large-
scale reservoir simulations on parallel systems and designing various data structures. The platform is implemented using C and MPI (Message Passing Interface). MPI is a standardized message-passing system designed to work on a wide variety of parallel systems and it is employed to handle communications among computation nodes. The platform provides structured grid, cell-centered data, linear solvers, preconditioners, distributed matrices and vectors, visualization, parallel input and output through MPI-IO, key words parsing and well modeling modules. Finite difference methods and finite volume methods are supported. The load balancing module is crucial for parallel computing \[34, 36, 24\]. The load balancing module is completed by ParMETIS \[36\] and the Hilbert space-filling curve (HSFC) method \[34\]. The ParMETIS is a graph partitioning package using topological information of a grid, and the HSFC partitioning method is an in-house partitioning method, which serves as the default partitioner. Commonly used Krylov subspace solvers and algebraic multigrid (AMG) solvers are implemented, including the restarted GMRES solver, BiCGSTAB solver \[12\], and classic AMG solvers \[33\]. General preconditioners, including ILU(k), ILUT, domain decomposition \[22\] and AMG \[33\], and special preconditioners, including CPR-like preconditioners, are implemented. Detailed designs and key parameters are presented. Numerical experiments show that our platform is capable of calculating problems with hundreds of millions of grid cells and it has excellent scalability on distributed-memory parallel computers.

2. Gridding and Data

A traditional reservoir can be described as \( \Omega = [x_1, x_2] \times [y_1, y_2] \times [z_1, z_2] \). If the domain \( \Omega \) are divided into \( n_x \), \( n_y \) and \( n_z \) intervals in the \( x, y \) and \( z \) directions, then the grid has \( N_g = n_x \times n_y \times n_z \) cells. Each cell is a hexahedron. An interior cell has six neighbors and each boundary cell may have three, four or five neighbors, depending on its location. A structured grid can be uniform or non-uniform. The structured grids support finite difference methods, finite volume methods and finite element methods, and they have been widely used by commercial reservoir simulators.

Data structures in this paper use C language style. Figure 1 presents our basic data types for integer, float-point, boolean and character types and MPI-related data types used by MPI. These data types are generated automatically by project management tools, such as autoconf and m4 language. They can also be redefined by configure options when being compiled. Dou-
typedef double FLOAT;
#if USE_LONG
typedef signed long int INT;
typedef unsigned long int UINT;
#else
typedef signed int INT;
typedef unsigned int UINT;
#endif
typedef unsigned short USHORT;
typedef char CHAR;
typedef FLOAT COORD[3]; /* space coordinates */
#ifndef TRUE
#define TRUE (1)
#endif
#ifndef FALSE
#define FALSE (0)
#endif
typedef int BOOLEAN;

/* MPI type */
#define PRSI_MPI_FLOAT MPI_DOUBLE
#if USE_LONG
#define PRSI_MPI_INT MPI_LONG
#define PRSI_MPI_UINT MPI_UNSIGNED_LONG
#else
#define PRSI_MPI_INT MPI_INT
#define PRSI_MPI_UINT MPI_UNSIGNED
#endif
#define PRSI_MPI_CHAR MPI_CHAR
#define PRSI_MPI_BOOLEAN MPI_INT

/* CSR format */
typedef struct mat_csr_t _ {
    INT num_rows;
    INT num_cols;
    INT num_nonzeros;
    INT *Ap;
    INT *Aj;
    FLOAT *Ax;
} mat_csr_t;

Figure 1: Basic data types

Figure 2: Basic data types

...ble precision is used for floating-point number and integer can be 32-bit and other types.

The data structure of a cell, which is defined as CELL, is shown by Figure 2. This data structure defines cell-related information, such as centroid coordinate (ctrd), area of all faces (area) and volume (vol), six neighbors (nb), local index of each vertex (vert), local index on an MPI process (index),...
typedef struct CELL_
{
    #if !USE_LESS_MEMORY
        COORD ctrd; /* centroid coordinate */
        FLOAT area[6]; /* area of each face */
        FLOAT vol; /* volume */
    #endif
    void *nb[6]; /* neighbours */
    INT vert[8]; /* local index of vertices */
    INT index; /* local index */
    INT idx[3]; /* index in x, y and z direction */
    INT regn; /* region mark */
    USHORT bdry_type[6]; /* boundary type */
    USHORT type; /* cell type */
} CELL;

Figure 2: Data structure of CELL

global index in three directions (idx), region mark (regn), boundary type of each face (bdry_type) and cell type (type). Some members are optional. For example, if we would like to use less memory, we can remove ctrd, area and vol by setting USE_LESS_MEMORY to some positive integer, such as 1. In reservoir simulations, each cell represents a portion of reservoir and they have similar properties, such as porosity, pressure, temperature, water saturation and oil saturation.

Each cell has a unique global index. Its default index is calculated as

\[ C_{(i,j,k)} = n_x * n_y * k + n_x * j + i, \]

which is numbered from the bottom layer of a reservoir to the top layer of the reservoir. Here \(i, j, k\) are the integer coordinates of the cell in the \(x, y, z\) directions, respectively. Another numbering style used by most reservoir simulators is

\[ C_{(i,j,k)} = n_x * n_y * (n_z - k) + n_x * j + i, \]

which is numbered from top layer to bottom layer.

Data structure for structured grids, GRID, is presented in Figure 3 which stores the coordinates of each vertex (vert), vertex indices (L2Gmap_vert), cell indices (L2Gmap_cell), distribution of cells (num_cells) in each MPI process, a mapping between the global index of a cell and its local index, well data and MPI info. In each MPI process, a portion of a grid is stored,
typedef struct GRID_
{
    COORD  *vert;    /* coordinates of each vertex */
    CELL   *cell;    /* number of cells in each process */
    INT    *num_cells;    /* remote neighbours */
    RNEIGH *rngbr;    /* vert types */
    USHORT *type_vert;    /* Local to global map of vertices */
    INT    *L2Gmap_vert;    /* Local to global map of cell indices */
    FLOAT  lif;    /* Load imbalance factor */
    INT    nregns;    /* number of region marks */
    INT    nfaces;    /* number of faces */
    INT    ncells;    /* number of cell indices in the subgrid */
    INT    nfaces_remote;    /* number of remote neighbours */
    INT    nverts;    /* number of vertices in the subgrid */
    INT    nfaces_global;    /* number of vertices in the global grid */
    INT    ncells_global;    /* number of cells in the global grid */
    INT    nfaces_remote;    /* equals to number of remote neighbours */
    INT    nverts_global;    /* number of vertices in the global grid */
    INT    nfaces_global;    /* number of faces */
    INT    ncells_global;    /* number of cells in the global grid */
    FLOAT  bbox[3][2];    /* bounding box */
    INT    ncx, ncy, ncz;    /* grid size in x, y, z directions */
    FLOAT  vx, vy, vz;    /* partition of x, y, and z directions */
    BOOLEAN uniform;    /* uniform in each direction or not */

    /* Well, (nprocs - 1)-th process owns all wells */
    WELL **well;
    WELL_CINFO *well_cinfo;
   CELL  **perf_cell;    /* pointer to cell which has perforation */
    INT    nperfs;    /* number of perforations */
    INT    nperfs_global;
    INT    nwells_global;    /* number of wells */
    BOOLEAN well_assembled;
    BOOLEAN destroy_well;    /* if grid or simulator destroy wells */

    MPI_Comm comm;
    int rank;
    int nprocs;
} GRID;

Figure 3: Data structure of GRID

and only vertices and faces belong to these cells are stored. Space cost of a
grid in each MPI process is proportional to grid size (number of cells).

When a neighbor of a cell is in another MPI process, communication is
required when accessing neighbor information. The data structure RNEIGH
stores remote cell information, such as its global cell index (gidx), its local
index (lidx), and its MPI rank (rank). The member rank defines message
sender and receiver during communication.
typedef struct RNEIGH_
{
    INT gidx;
    INT lidx;
    int rank;
} RNEIGH;

Figure 4: Data structure of remote neighbor

2.1. Grid Partitioning

Let $G$ be the structured grid, which is distributed in $N_p$ MPI tasks,

$$G = \{C_1, C_2, \cdots, C_{N_g}\},$$

where $C_i$ is the $i$-th cell of $G$. Each task owns a subset of $G$, $G_i$, which satisfies the following conditions:

$$\begin{align*}
    G_i &\neq \emptyset \ (i = 1, \cdots, N_p) \\
    G_i \cap G_j &\neq \emptyset \ (i \neq j) \\
    \cup G_i &= G \ (i = 1, \cdots, N_p).
\end{align*}$$

A cell belongs to some sub-grid, and its neighboring cells may belong to different sub-grids.

Each cell has similar calculations. Therefore, it is seasonable to assume that each cell has the same amount of calculations. The workload of each MPI task can be modeled by the size of its sub-grid, $|G_i|$, or simply the number of grid cells in the sub-grid. When discretizing reservoir models, information from neighboring cells is always required. For any sub-grid, its communication volume is determined by its remote neighboring cells, which can be modeled by dual graph: we see a cell as a vertex of a graph, and if two cells are neighbors, there exists an edge between these two cells. The dual graph can be presented by a sparse matrix, such as a CSR (Compressed Sparse Row) matrix.

The goal of grid partitioning is that each MPI task has equal workload (number of cells) and the communications are minimized. We have mentioned that communications can be modeled by dual graph. Graph partitioning packages, such as ParMETIS, are ideal tools. The geometry information based methods are also efficient, including recursive coordinate bisection method, recursive inertial bisection method and the space-filling curve methods [34]. We implement the Hilbert space-filling curve method as the default
partitioning method, since Hilbert space-filling curves have better spatial locality than other space-filling curves, such as Morton space-filling curves.

### 2.2. Data

The cell-centered data is natural to reservoir simulation, since each cell can represent a block of a real oil and gas field and we can attach properties to the cell. Its data structure, **DOF**, is shown in Figure 5.

```c
typedef struct DOF_TYPE_
{
  INT np_cell; /* number of DOFs per cell */
  INT np_well; /* number of DOFs per well */
} DOF_TYPE;

typedef struct DOF_
{
  char *name; /* name of DOF */
  GRID *g; /* the grid */
  DOF_TYPE *type; /* type of DOF */
  FLOAT *data;
  INT *idata;
  INT count_cell; /* data count per cell */
  INT count_well; /* data count per well */
  INT count_perf; /* data count per perforation */
  INT dim;
  BOOLEAN assembled;
} DOF;
```

**Figure 5:** Data structure of DOF

Each **DOF** has a name (**name**), and it associates with a grid (**g**). It also has a type (**type**). It can define floating-point number and integer data. A **DOF** also has a dimension (**dim**), through which scalar and vector can be defined. In reservoir simulations, cells have different properties, such as oil and water saturations, porosity and permeability. It is straightforward to define **DOF_TYPE_CELL**, which associates with each cell. A **DOF** has a member **dim**, which defines dimension of a **DOF**. It can be scalar (one dimension) or vector (multiple dimension). **DOF_TYPE_WELL** defines data for each well in a grid. One well may perforate several cells and some properties only exist on these perforated cells, such as oil production rate and water injection rate. We have another type, **DOF_TYPE_PERF**, which has value on all perforated cells only.
Input and output (reading data from a file and writing data to a file) for sequential applications are trivial, and simple writing and reading functions from operating systems or C language are enough. However, when we are working on parallel computing, each MPI task has portion of the whole grid and portion of data, and each task only reads and writes part of data. If each MPI task reads the whole input file and picks necessary data, then most read data will be dropped and they compete disk with each other. If all MPI tasks write data to the same file, conflicts may exist. The platform provides parallel input and output modules using MPI-IO, which supports integer and floating-point numbers.

The initialization of reservoir simulations requires read reservoir properties from files, such as porosity and permeability. The restart of simulations also needs to write intermediate data and to read data files. They are achieved by our parallel input and output modules.

3. Distributed Matrices and Vectors

A linear system, $Ax = b$ ($A \in R^{N \times N}$), is assembled in each Newton iteration. Distributed matrix and vector are required to store the linear system. In the platform, each matrix and vector are distributed among all MPI tasks.

Each row of the distributed matrix has a unique global row index, which ranges from 0 to $N - 1$ consecutively and is numbered from the 1-th MPI task to the $N_p$-th MPI task. Each row also has a local index on each MPI task. The global indices of a vector is numbered the same way.

A map, MAP, is defined to store communication information among cell data, matrices and vectors. It includes DOF information, off-process entries, communication pattern, locations of data required by other MPI tasks and locations of data received from other MPI tasks.

A distributed floating-point vector is defined in Figure 6 which has buffer that holds data entries (data), number of local entries belong to current MPI task (nlocal), number of total entries (including off-process entries, localsize) and reference to mapping information.

The data structure of a distributed matrix is more complex than a vector, which requires entries for each row and some other additional information. It is represented in Figure 7. The MAT_ROW stores non-zero entries of each row and its storage format is similar to a CSR matrix, which has a value of an entry (data), the global index (gcol) and local index of an entry (col).
typedef struct VEC_
{
    MAP *map;
    FLOAT *data;
    INT nlocal; /* entries belong to current proc */
    INT localsize; /* total entries in current MPI process */
} VEC;

Figure 6: Data structure of VEC

typedef struct MAT_ROW_
{
    FLOAT *data; /* data */
    INT *cols; /* local column indices, INT[ncols] */
    INT *gcols; /* global column indices, INT[ncols] */
    INT ncols; /* number of nonzero columns */
} MAT_ROW;

typedef struct MAT_
{
    MAT_ROW *rows;
    MAP *map;
    COMM_INFO *cinfo;
    INT *O2Gmap;
    INT nlocal; /* local entries belong to current proc */
    INT localsize; /* total local entries */
    INT nglobal; /* global matrix size */
    INT *part; /* distribution information */
    int rank;
    int nprocs;
    MPI_Comm comm;
    BOOLEAN assembled;
} MAT;

Figure 7: Data structure of MAT

The MAT has communication information (cinfo), MPI information and additional information, such as mapping between local index of off-process entries and their global indices (O2Gmap), and row distribution among all MPI tasks (part).

Figure shows communication info used by matrix and vector. This data structure can be used for collection communications, such as MPI_Alltoallv, and point-to-point communications. scnts means data amounts sent by current MPI task to other MPI tasks, and sdsps means the displacement.
typedef struct COMM_INFO_
{
    INT *sidx;
    INT *widx;
    int *scnts, *sdsps;
    int *rcnts, *rdsps;
    MPI_Comm comm;
    INT ssize, rsize;
} COMM_INFO;

Figure 8: Data structure of communication info

relative to sending buffer. rcnts means data amounts received from other MPI tasks, and rdsps is the displacement relative to receiving buffer. ssize is total data sent by current MPI task and rsize is total received data. sidx is the index of data to be sent. widx is the local index of data received in current MPI task.

With the help of above data structures, commonly used matrix-vector operations and vector operations can be implemented directly, which are listed as follows:

\[ y = \alpha Ax + \beta y, \]  
\[ z = \alpha Ax + \beta y, \]  
\[ y = \alpha x + \beta y, \]  
\[ z = \alpha x + \beta y, \]  
\[ \alpha = \langle x, y \rangle, \]  
\[ \alpha = \langle x, x \rangle^{\frac{1}{2}}, \]

where \( A \) is a matrix, \( \alpha \) and \( \beta \) are scalars, and \( x \) and \( y \) are vectors.

4. Linear System

For the linear system, \( Ax = b \), derived from a nonlinear method, Krylov subspace solvers including the restarted GMRES(m) solver, the BiCGSTAB solver, and algebraic multi-grid (AMG) solvers are commonly used to find
its solution. The Krylov subspace solvers mentioned here are suitable for arbitrary linear systems while the algebraic multi-grid solvers are efficient for positive definite linear systems.

4.1. Solvers

In-house parallel Krylov subspace linear solvers are implemented. The data structure of our solvers, SOLVER, is shown in Figure 9 which includes parameters \((\text{rtol}, \text{atol}, \text{btol}, \text{maxit}, \text{restart})\), matrices, right-hand sides, solutions, and preconditioner information.

The data structure SOLVER\_API defines a framework, which stores interfaces for solver creation, destroying, entries adding, assembling and solutions. Other solvers can be coupled with our platform right away.

4.2. Preconditioners

Several preconditioners are developed, including general purpose preconditioners and physics-based preconditioners for reservoir simulations only.

4.2.1. Restricted Additive Schwarz Method

For the classical ILU methods, the given matrix \(A\) is factorized into a lower triangular matrix \(L\) and an upper triangular matrix \(U\); a lower triangular linear system and an upper triangular linear system are required to solve:

\[
LUx = b \iff Ly = b, Ux = y.
\]

The systems need to be solved row-by-row, which are serial. It is well-known that they have limited scalability. Another option for parallel computing is the restricted additive Schwarz (RAS) method [20], which was developed by Cai et al.

The data structure of the RAS preconditioner is shown in Figure 10. The \texttt{pars} stores parameters of the RAS preconditioner, such as overlap, local solver (ILUK, ILUT and ILTC), the level of ILUK, memory control and tolerance of ILUT, and filter tolerance. The \texttt{RAS\_DATA} has a local problem stored by the lower triangular matrix \(L\) and the upper triangular matrix \(U\), communication information of different sub-domains (\texttt{cinfo}), memory buffer and prolongation (restriction) operation information.

The default parameters of the RAS preconditioner is shown in Figure 11. Its default local solver is ILU(0). Default parameters for ILUT(\(p\), \(tol\)) is -1 and 1e-3. If \(p\) is -1, the factorization subroutine will determine dynamically.
4.2.2. Algebraic Multigrid Methods

If $A$ is a positive-definite square matrix, the AMG methods \cite{31, 30, 27, 28, 29, 2} have proved to be efficient methods and they are also scalable \cite{21}. AMG methods have hierarchical structures, and a coarse grid is chosen when entering a coarser level. The Cleary-Luby-Jones-Plassman (CLJP) parallel coarsening algorithm was proposed by Cleary \cite{23} based on the algorithms developed by Luby \cite{26} and Jones and Plassman \cite{25}. The standard RS coarsening algorithm has also been parallelized \cite{33}. Falgout et al. de-
typedef struct RAS_PARS_
{
    INT overlap;
    INT iluk_level;
    INT ilut_p;
    int solver;
    FLOAT ilut_tol;
    FLOAT filter_tol;
    INT ilutc_drop;
} RAS_PARS;

typedef struct RAS_DATA_
{
    COMM_INFO *cinfo;
    mat_csr_t L;
    mat_csr_t U;
    FLOAT *frbuf;
    FLOAT *fxbuf;
    FLOAT *fbbuf;
    INT *ras_pro; /* ras prolongation */
    INT num_ras_pro;
    RAS_PARS pars;
} RAS_DATA;

static RAS_PARS ras_pars_default =
{
    /* overlap */ 1,
    /* k */ 0,
    /* ilut_p */ -1,
    /* solver */ ILUK,
    /* ilut_tol */ 1e-3,
    /* filter tol */ 1e-4,
    /* drop */ 0,
};

In our platform, the AMG solvers are from HYPRE. They can be used as solvers and preconditioners. The data structure of the AMG solvers is
typedef struct BMAMG_PARS_
{
    INT maxit;
    INT num_funcs; /* size of the system of PDEs */
    INT max_levels; /* max MG levels */
    FLOAT strength; /* strength threshold */
    FLOAT max_row_sum; /* max row sum */
    FLOAT trunc_tol; /* trunc tol */
    int coarsen_type; /* default coarsening type = Falgout */
    int cycle_type; /* MG cycle type */
    int relax_type; /* relaxation type */
    int coarsest_relax_type; /* relax type on the coarsest grid */
    int interp_type; /* interpolation */
    INT num_relax; /* number of sweep */
} BMAMG_PARS;

typedef struct BMAMG_DATA_
{
    MAP *map;
    INT ilower, iupper;
    HYPRE_IJMatrix A;
    HYPRE_IJVector b, x;
    BOOLEAN assembled;
    HYPRE_Solver hsolver;
    SolveFcn setup;
    SolveFcn solve;
    DestroyFcn destroy;
    BMAMG_PARS pars;
} BMAMG_DATA;

Figure 12: Data structure of AMG method

shown in Figure12. The BMAMG_PARS stores parameters of the AMG method, including the coarsening type, interpolation type, maximal levels, smoother type, and cycle type. The BMAMG_DATA stores linear system information, such as a distribution pattern of matrices and vectors, mapping information, and related interfaces.

Default parameters for the AMG method is shown in Figure13, where a default six-level AMG method is applied. The detailed explanation of each parameter can be read from the HYPRE user manual.

4.2.3. CPR-like Preconditioners

Linear systems from black oil and composition models are hard to solve, especially when the reservoirs are heterogeneous. However, the matrices from the pressure unknowns are positive definite, which can be solved by AMG
methods. Many preconditioners have been developed to speed the solution of linear systems, such as the constrained pressure residual (CPR) method and FASP method [18]. Here we introduce our multi-stage preconditioners for the black oil and compositional models, which are based on the classical CPR method.

Numerical methods for black oil and compositional models may choose different unknowns [32]. Here we assume that the oil phase pressure $p_o$ is always one of the unknowns. The other variables are denoted as $\mathbf{s}$. The well unknowns are denoted as $\mathbf{w}$, whose dimension equals the number of wells in the reservoir, $N_w$. Let us define the pressure vector $p$ as:

$$p = \begin{pmatrix} p_{o,1} \\ p_{o,2} \\ \vdots \\ p_{o,N_o} \end{pmatrix},$$

(12)
and the global unknown vector $x$ as:

$$
    x = \begin{pmatrix}
        p_{o,1} \\
        p_{o,2} \\
        \vdots \\
        p_{o,N_g} \\
        s_1^g \rightarrow \cdot \cdot \cdot \\
        \vdots \\
        s_{N_g}^g \rightarrow \cdot \cdot \cdot \\
        \bar{w}
    \end{pmatrix},
$$

(13)

A restriction operator from $x$ to $p$ is defined as

$$
    \Pi_r x = p.
$$

(14)

A prolongation operator $\Pi_p$ is defined as

$$
    \Pi_p p = \begin{pmatrix}
        p \\
        0
    \end{pmatrix},
$$

(15)

where $\Pi_p p$ has the same dimension as $x$.

If a proper ordering technique is applied, the matrix $A$ from black oil and compositional models can be written as equation (16),

$$
    A = \begin{pmatrix}
        A_{pp} & A_{ps} & A_{pw} \\
        A_{sp} & A_{ss} & A_{sw} \\
        A_{wp} & A_{ws} & A_{ww}
    \end{pmatrix},
$$

(16)

where the sub-matrix $A_{pp}$ is the matrix corresponding to the pressure unknowns, the sub-matrix $A_{ss}$ is the matrix corresponding to the other unknowns, the sub-matrix $A_{ww}$ is the matrix corresponding to the well bottom hole pressure unknowns, and other matrices are coupled items.

Let us introduce some notations for the preconditioning system $Ax = f$. If $A$ is a positive definite matrix, then we define the notation $M_g(A)^{-1} b$ to represent the solution $x$ from AMG methods. If it is solved by the RAS method, then we use the notation $R(A)^{-1} b$ to represent solution $x$. The CPR-like preconditioners we develop are shown by Algorithm [1] and Algorithm [2] which are noted as CPR-FP and CPR-FPF [40], respectively.
**Algorithm 1** The CPR-FP preconditioner

1: \( x = \mathcal{R}(A)^{-1} f. \)
2: \( r = f - Ax \)
3: \( x = x + \Pi_p(\mathcal{M}_p(A_{pp})^{-1}(\Pi_r r)). \)

**Algorithm 2** The CPR-FPF preconditioner

1: \( x = \mathcal{R}(A)^{-1} f. \)
2: \( r = f - Ax \)
3: \( x = x + \Pi_p(\mathcal{M}_p(A_{pp})^{-1}(\Pi_r r)). \)
4: \( r = f - Ax \)
5: \( x = x + \mathcal{R}(A)^{-1} r. \)

```c
typedef struct CPR_PARS_
{
    RAS_PARS ras;
    BMAMG_PARS amg;
    INT pres_which;
    INT pres_loc;
    INT itr_ras_pre;
    INT itr_ras_post;
} CPR_PARS;

typedef struct CPR_DATA_
{
    RAS_DATA ras;
    BMAMG_DATA amg;
    INT *pro_pres; /* prolongation from pressure */
    INT num_pro_pres;
    VEC *varbuf; /* vector r (A), buffer */
    VEC *vpbbuf; /* buffer for AMG */
    VEC *vpxbuf; /* buffer for AMG */
    CPR_PARS pars;
} CPR_DATA;
```

Figure 14: Data structure of CPR preconditioners

The data structure of the CPR preconditioners is shown in Figure 14. It has a RAS solver (ras) an AMG solver (amg), prolongation information (pro_pres) and num_pro_pres, buffers and settings for RAS solver and AMG solver. The term CPR_PARS stores parameters of the CPR methods.
4.3. Data Structure for Preconditioners

The data structure for preconditioners is defined by Figure 15. It provides three function pointers that can complete assembling (PC_USER_ASSEMBLE), solving (PC_SOLVE) and destroying (PC_DESTROY) a preconditioning system. With these function pointers, this data structure is general purpose, and if a new set of implementations are provided, a new preconditioner can be constructed. From the data structure, we can see built-in preconditioners, including RAS method, AMG methods and CPR methods, are provided, and users can implement their own preconditioners by providing proper assembling, solving and destroying functions. The data structure also contains a pointer to solver, and MPI info.

```c
/* pc type */
typedef enum PC_TYPE_
{
    PC_RAS,    /* Restricted Additive Schwarz */
    PC_AMG,    /* BommerAMG */
    PC_CPR,    /* CPR */
    PC_USER,   /* user define */
    PC_NON,    /* no preconditioner */
} PC_TYPE;

/* preconditioner interface */
typedef void (*PC_USER_ASSEMBLE)(struct SOLVER_PC_ *pc, MAT *mat);
typedef void (*PC_SOLVE)(struct SOLVER_PC_ *pc, VEC *x, VEC *b);
typedef void (*PC_DESTROY)(struct SOLVER_PC_ *pc);

/* SOLVER_PC struct */
typedef struct SOLVER_PC_
{
    struct SOLVER_ *solver;    /* pointer to solver */
    void *data;
    PC_USER_ASSEMBLE user_assemble;
    int rank;
    int nprocs;
    MPI_Comm comm;
    PC_SOLVE solve;
    PC_DESTROY destroy;
    BOOLEAN assembled;
} SOLVER_PC;
```

Figure 15: Data structure of preconditioners
5. Numerical Experiments

A Blue Gene/Q from IBM that located in the IBM Thomas J. Watson Research Center is employed. The system uses PowerPC A2 processor. Each processor has 18 cores and 16 cores are used for computation. Performance of each core is really low compared with processors from Intel. However, it has a strong network relative to compute performance and the system is scalable. Since the platform is designed for parallel applications, scalability is the most important objective. In the following section, we will focus on scalability.

5.1. SpMV

**Example 1.** This example tests the performance of sparse matrix-vector multiplication (SpMV) on IBM Blue Gene/Q. The matrix is a square matrix from a Poisson equation and it has 200 millions rows. Its performance is shown in Table 1 and its scalability is presented in Figure 16.

| # proc  | 32  | 64  | 128 | 256 | 512 | 1024 |
|---------|-----|-----|-----|-----|-----|------|
| Time (s)| 2.211 | 1.078 | 0.556 | 0.269 | 0.134 | 0.067 |

Table 1: Performance of SpMV, Example 1

![Figure 16: Scalability of SpMV, Example 1](image)
This example uses up to 128 compute cards, when more than 128 MPI tasks are used, multiple MPI tasks run on one card. From Table 1, we can see that when MPI tasks are doubled, the running time of SpMV is reduced by half. This example show our SpMV kernel has excellent scalability. Speedup is compared with ideal condition in Figure 16, which shows that our SpMV kernel has good scalability.

5.2. Poisson Equation

**Example 2.** This example tests a Poisson equation with 3 billions of grid cells. The example uses up to 4,096 CPU cores (MPIs). The linear solver is GMRES(30) method with RAS preconditioner. The solver runs 90 iterations. The overlap of RAS method is one, and sub-domain problem on each core is solved by ILU(0). The numerical summaries are reported in Table 2 and scalability results are shown in Figure 17.

| # proc  | Gridding | Building | Assemble | Overall (s) | Speedup |
|---------|----------|----------|----------|-------------|---------|
| 512     | 217.0    | 29.16    | 66.42    | 918.91      | 1.0     |
| 1024    | 98.83    | 14.79    | 33.71    | 454.04      | 2.02    |
| 2048    | 47.53    | 7.49     | 17.47    | 227.05      | 4.05    |
| 4096    | 23.31    | 3.86     | 9.17     | 116.64      | 7.88    |

Table 2: Numerical summaries of Example 2

Table 2 shows numerical summaries of Poisson equation. This example tests strong scalability of our platform. Here the gridding time includes grid generation, grid partitioning and grid redistribution. From Table 2, we can see that the gridding has excellent scalability and when MPIs are doubled, running time for gridding reduces by half. Building time is the time spent on generation of a linear system $Ax = b$. Since there is no communication involved, the scalability is ideal. Assemble time includes time for generating linear solver, and time for generating preconditioner (RAS method). The overall time includes gridding time, building time, assemble time and solution time. Again, from Table 2 and Figure 17, we can see our platform has excellent scalability.

5.3. Oil-water Model

**Example 3.** This example tests a refined SPE10 case for the two-phase oil-water model, where each grid cell is refined into 27 grid cells. This case has
around 30 millions of grid cells and around 60 millions of unknowns. The stopping criterion for the inexact Newton method is $10^{-3}$ and the maximal Newton iterations are 20. The BiCGSTAB solver is applied and its maximal iterations are 100. The preconditioner is the CPR-FPF preconditioner. The potential reordering and the Quasi-IMPES decoupling strategy are applied. The simulation period is 10 days. Up to 128 compute cards are used. The numerical summaries are shown in Table 3, and the speedup (scalability) is shown in Figure 18.

| # procs | # Steps | # Ntn | # Slv | Avg-S | Time (s) | Avg-T (s) |
|---------|---------|-------|-------|-------|----------|-----------|
| 64      | 50      | 315   | 3451  | 10.9  | 119167.4 | 378.3     |
| 128     | 48      | 286   | 3296  | 11.5  | 49488.7  | 173.0     |
| 256     | 54      | 323   | 4190  | 12.9  | 30423.2  | 94.1      |
| 512     | 52      | 329   | 3635  | 11.0  | 14276.5  | 43.3      |
| 1024    | 54      | 316   | 3969  | 12.5  | 7643.9   | 24.1      |

Table 3: Numerical summaries of Example 3

In this example, up to 1,024 MPI tasks are employed and the simulation with 64 MPI tasks is used as the base case to calculate speedup and scalability. The numerical summaries in Table 3 show the inexact Newton
method is robust, where around 50 time steps and around 300 Newton iterations are used for each simulation with different MPI tasks. The linear solver BiCGSTAB and the preconditioner CPR-FPF show good convergence, where the average number of linear iterations for each nonlinear iteration is between 10 and 13. The results mean our linear solver and preconditioner are effective and efficient. The overall running time and average time for each Newton iteration show our simulator has excellent scalability on IBM Blue Gene/Q, which is almost ideal for parallel computing. The scalability is also demonstrated in Figure 18. The running time and scalability curve also demonstrate our linear solver and preconditioner are scalable for large-scale simulation.

Example 4. This example tests a refined SPE10 case for the two-phase oil-water model, where each grid cell is refined into 125 grid cells. This case has around 140 millions of grid cells and around 280 millions of unknowns. The stopping criterion for the inexact Newton method is 1e-2 and the maximal Newton iterations are 20. The GMRES(30) solver is applied and its maximal iterations are 100. The preconditioner is the CPR-FPF preconditioner. The potential reordering and the Quasi-IMPES decoupling strategy are applied. The simulation period is 2 days. Up to 128 compute cards are used. The numerical summaries are shown in Table 4, and the speedup (scalability) is shown in Figure 19.
In this example, up to 2048 MPI tasks are employed and the simulation with 256 MPI tasks is used as the base case to calculate speedup and scalability. The numerical summaries in Table 4 show the inexact Newton method is robust, where around 36 time steps and around 220 Newton iterations are used for each simulation with different MPI tasks. The linear solver GMRES(30) and the preconditioner CPR-FPF show good convergence, where the average number of linear iterations for each nonlinear iteration is around 26. The overall running time and average time for each Newton iteration show our simulator has excellent scalability on IBM Blue Gene/Q, which is almost ideal for parallel computing and shows slight super-linear scalability. The scalability is also demonstrated in Figure 19. The results show our linear solver and preconditioner are scalable for large-scale simulation.
5.4. Black Oil Model

Example 5. The example tests the scalability of the black oil simulator using a refined SPE10 geological model, where each grid cell is refined to 27 grid cells. The model has 30.3 millions of grid cells. The inexact Newton method is applied and the termination tolerance is $10^{-2}$. The linear solver is BiCGSTAB, whose maximal inner iterations are 100. The preconditioner is the CPR-FPF method and the overlap for the RAS method is one. The potential reordering and the ABF methods are enabled. The simulation period is 10 days. The maximal change allowed in one time step of pressure is 1,000 psi and the maximal change of saturation is 0.2. Up to 128 compute cards are used. Summaries of numerical results are shown in Table 5.

| # procs | # Steps | # Ntn | # Slv | Avg-S | Time (s) |
|---------|---------|-------|-------|-------|----------|
| 64      | 33      | 292   | 1185  | 4.0   | 106265.9 |
| 128     | 33      | 296   | 1150  | 3.8   | 50148.3  |
| 256     | 33      | 299   | 1267  | 4.2   | 25395.8  |
| 512     | 33      | 301   | 1149  | 3.8   | 12720.5  |
| 1024    | 33      | 301   | 1145  | 3.8   | 6814.2   |

Table 5: Numerical summaries of Example 5

![Figure 20: Scalability (speedup) of Example 5](image-url)
Table 5 includes information for the nonlinear method, linear solver and running time. For all simulations, 33 time steps are used and the total Newton iterations are around 300. The results show the inexact Newton method is robust. For the linear solver and preconditioner, their convergence is good, which terminate in around 4 iterations. The results mean the linear solver and preconditioner are robust and effective for this highly heterogeneous model. The running time, average time per Newton iteration and scalability curve in Figure 20 show the scalability of our simulator, linear solver and preconditioner is good. When we use up to 1,024 MPI tasks and each compute card runs up to 8 MPI tasks, the scalability is excellent.

Example 6. The case is a refined SPE1 project with 100 millions of grid cells. Linear solver is BiCGSTAB. Potential reordering and ABF decoupling are applied. Numerical summaries are in Table 6.

| MPIs | # Steps | # Newton | # Solver | # Avg. Itr | Time (s) |
|------|---------|----------|----------|------------|----------|
| 512  | 27      | 140      | 586      | 4.1        | 11827.9  |
| 1024 | 27      | 129      | 377      | 2.9        | 5328.4   |
| 2048 | 26      | 122      | 362      | 2.9        | 2708.5   |
| 4096 | 27      | 129      | 394      | 3.0        | 1474.2   |

Table 6: Numerical summaries, Example 6

6. Conclusion

Our work on developing an in-house parallel platform is presented in this paper, which provides grids, data, linear solvers and preconditioners for reservoir simulators. Various techniques and methods have been introduced, including the Hilbert space-filling curve method, topological partitioning method, structured grid, distributed matrices and vectors, and multi-state preconditioners for reservoir simulations. Examples, including grid management, linear solvers, pressure equations, and the black oil simulator, are presented to benchmark our platform. Numerical results show that our platform and simulators have excellent scalability and applications based on the platform can be sped up thousands of times faster. This paper also shows parallel computing is a powerful tool for large-scale scientific computing.
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