Understanding Breakthrough Curves

v0.1

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Chapter 1

Todo List

Class Variables_j

Change c_j and c_jm1 to a_j and a_jm1 to reflect notation change in paper

Chapter 2

Data Structure Index

2.1 Data Structures

Here are the data structures with brief descriptions:

Chapter 3

File Index

3.1 File List

Here is a list of all documented files with brief descriptions:

Chapter 4

Data Structure Documentation

4.1 AppCtx Struct Reference

Useful parameters for solving, Application context.

```
#include <my_petsc.h>
```

Collaboration diagram for AppCtx:

Data Fields

- PetscInt j
- PetscInt m
- PetscReal errnorm_all
- PetscReal eps
- ISO isotherm
- PetscReal theta
- PetscReal dx
- PetscReal dtau
- PetscReal ∗ btc
- PetscReal tau_star
- VecAndArray f_jm1
- VecAndArray S_jm1
- bool compute_analytical
- bool make_movie
- bool save_btc
- bool print_header
- PetscViewer viewer
- PetscInt movie_step_interval
- PetscReal omega
- PetscReal b
- PetscReal K
- PetscReal beta
- PetscReal kappa
- PetscReal dtau_est

4.1.1 Detailed Description

Useful parameters for solving, Application context.

4.1.2 Field Documentation

4.1.2.1 b

`PetscReal AppCtx::b`

scale factor for beta

4.1.2.2 beta

`PetscReal AppCtx::beta`

constant calculated

4.1.2.3 btc

`PetscReal* AppCtx::btc`

array for break-through curve

4.1.2.4 compute_analytical

`bool AppCtx::compute_analytical`

Whether or not to compute analytical solution

4.1.2.5 dtau

`PetscReal AppCtx::dtau`

time step

4.1.2.6 dtau_est

`PetscReal AppCtx::dtau_est`

estimated dtau for setting it when tau_star unknown

4.1.2.7 dx

```
PetscReal AppCtx::dx
```

grid spacing

4.1.2.8 eps

```
PetscReal AppCtx::eps
```

value of ε

4.1.2.9 errnorm_all

```
PetscReal AppCtx::errnorm_all
```

infinity norm

4.1.2.10 f_jm1

```
VecAndArray AppCtx::f_jm1
```

Isotherm function at previous time step

4.1.2.11 isotherm

```
ISO AppCtx::isotherm
```

structure for adsorption isotherm

4.1.2.12 j

```
PetscInt AppCtx::j
```

time step

4.1.2.13 K

```
PetscReal AppCtx::K
```

scale factor for kappa

4.1.2.14 kappa

```
PetscReal AppCtx::kappa
```

constant calculated

4.1.2.15 m

`PetscInt AppCtx::m`

total number of steps

4.1.2.16 make_movie

`bool AppCtx::make_movie`

whether or not to make movie

4.1.2.17 movie_step_interval

`PetscInt AppCtx::movie_step_interval`

step interval for saving movie frames

4.1.2.18 omega

`PetscReal AppCtx::omega`

closeness to steady state at end of simulation

4.1.2.19 print_header

`bool AppCtx::print_header`

whether to print header when displaying results of simulation

4.1.2.20 S_jm1

`VecAndArray AppCtx::S_jm1`

Solid concentration at previous time step

4.1.2.21 save_btc

`bool AppCtx::save_btc`

flag to save btc

4.1.2.22 tau_star

`PetscReal AppCtx::tau_star`

total simulation time $\tau_\star$

4.1.2.23 theta

```
PetscReal AppCtx::theta
```

fraction of BFD/FFD

4.1.2.24 viewer

```
PetscViewer AppCtx::viewer
```

petsc viewer

The documentation for this struct was generated from the following file:

- src/my_petsc.h

4.2 EXP_ISO Struct Reference

Data Fields

- double ∗ c_star
- double ∗ f_star
- int n
- double c_scale
- double f_scale

4.2.1 Field Documentation

4.2.1.1 c_scale

```
double EXP_ISO::c_scale
```

scale factor for concentration, multiplying c_scale by c_star gives units of mol/m3

4.2.1.2 c_star

```
double* EXP_ISO::c_star
```

scaled fluid concentration

4.2.1.3 f_scale

```
double EXP_ISO::f_scale
```

scale factor for loading, multiplying f_scale by f_star gives units of mol/m3

4.2.1.4 f_star

```
double* EXP_ISO::f_star
```

scaled solid concentration

4.2.1.5 n

```
int EXP_ISO::n
```

number of points

The documentation for this struct was generated from the following file:

- src/isotherm.h

4.3 ISO Struct Reference

Data Fields

- Fun F
- dFun dF
- int num_params
- double ∗ params
- double ∗ data

4.3.1 Field Documentation

4.3.1.1 data

```
double* ISO::data
```

data used for splines

4.3.1.2 dF

```
dFun ISO::dF
```

derivative of adsorption isotherm

4.3.1.3 F

```
Fun ISO::F
```

adsorption isotherm

4.3.1.4 num_params

```
int ISO::num_params
```

number of parameters used

4.3.1.5 params

```
double* ISO::params
```

parameters fit

The documentation for this struct was generated from the following file:

- src/isotherm.h

4.4 isotherm Struct Reference

The documentation for this struct was generated from the following file:

- src/isotherm.h

4.5 isotherm Struct Reference

The documentation for this struct was generated from the following file:

- src/isotherm.h

4.6 isotherms.Langmuir Class Reference

Public Member Functions

- def **__init__** (self, k)
- def **f** (self, c)
- def **df_dc** (self, c)
- def **s** (self, c)
- def **get_c_rarefaction** (self, x, t)
- def **get_c_shock** (self, x, t)
- def **is_rarefaction_wave** (self)
- def **is_shock_wave** (self)
- def **shock_lambda** (self)
- def **get_c_local_equilibrium** (self, x, t)

Data Fields

- **k**
- **name**

The documentation for this class was generated from the following file:

- src/isotherms.py

4.7 isotherms.Linear Class Reference

Public Member Functions

- def **__init__** (self)
- def **f** (self, c)
- def **df_dc** (self, c)

Data Fields

- **name**

The documentation for this class was generated from the following file:

- src/isotherms.py

4.8 Variables_j Struct Reference

Analytical and numerical variables at time j (and jm1 if analytical)

```
#include <my_petsc.h>
```

Collaboration diagram for Variables_j:

Data Fields

- VecAndArray W_j
- VecAndArray c_j
- VecAndArray c_jm1
- Vec error

4.8.1 Detailed Description

Analytical and numerical variables at time j (and jm1 if analytical)

Todo Change c_j and c_jm1 to a_j and a_jm1 to reflect notation change in paper

4.8.2 Field Documentation

4.8.2.1 c_j

`VecAndArray Variables_j::c_j`

Analytical values of fluid concentration at time j

4.8.2.2 c_jm1

`VecAndArray Variables_j::c_jm1`

Analytical values of fluid concentration at time $j-1$

4.8.2.3 error

`Vec Variables_j::error`

vector comprising errors (presumably b/t analytical and numerical)

4.8.2.4 W_j

`VecAndArray Variables_j::W_j`

Numerical values of fluid concentration at time j

The documentation for this struct was generated from the following file:

- src/my_petsc.h

4.9 VecAndArray Struct Reference

`#include <my_petsc.h>`

Data Fields

- Vec vec
- PetscReal $*$ arr

4.9.1 Detailed Description

Used for converting between vector and array types

4.9.2 Field Documentation

4.9.2.1 arr

```
PetscReal* VecAndArray::arr
```

array part

4.9.2.2 vec

```
Vec VecAndArray::vec
```

vector part

The documentation for this struct was generated from the following file:

- src/my_petsc.h

Chapter 5

File Documentation

5.1 src/isotherm.h File Reference

Functions and structs for adsorption isotherm.

```
#include <petsc.h>
```

Include dependency graph for isotherm.h:

5.2 src/my_funcs.hpp File Reference

For calculating analytical solutions.

Functions

- double exp_I0 (double T, double z)

  Calculate exponential term involving bessel function.
- double integrate (double T_jm1, double T_j, double z)

  Integrate expI0 from T_jm1 to T_j.
- double update_solution (double ∗c_j, double ∗c_jm1, double T_jm1, double T_j, double ∗X, int n)

  Updates solution from previous time step.
- void analytical_btc (double ∗, double ∗, double X, int)

  Provides analytical break-through curve.

5.2.1 Detailed Description

For calculating analytical solutions.

Used to calculate analytical solutions or break-through curves

Author

Robert F. DeJaco

5.2.2 Function Documentation

5.2.2.1 analytical_btc()

```
void analytical_btc (
             double * c,
             double * T,
             double X,
             int m )
```

Provides analytical break-through curve.

Parameters

c	fluid concentration
T	times
X	value for distance (1/epsilon)
m	number of times including 0

Returns

void

5.2.2.2 exp_I0()

```
double exp_I0 (
             double T,
             double z )
```

Calculate exponential term involving bessel function.

Evaluates $e^{-z-T} I_0(2\sqrt{zT})$, where I_0 is the modified Bessel function of zeroth order.

Parameters

T	Scaled value for time
z	Scaled value for distance

Returns

value of expression

5.2.2.3 integrate()

```
double integrate (
            double T_jm1,
            double T_j,
            double z )
```

Integrate expI0 from T_jm1 to T_j.

Evaluates

$$\int_{T_{j-1}}^{T_j} e^{-z-t} I_0\left(2\sqrt{zt}\right)\, dt$$

See also

exp_I0

Parameters

T_jm1	scaled time at previous index j-1
T_j	scaled time at current/next index j
z	scaled distance

Returns

value of expression

5.2.2.4 update_solution()

```
double update_solution (
            double * c_j,
            double * c_jm1,
            double T_jm1,
            double T_j,
            double * X,
            int n )
```

Updates solution from previous time step.

Parameters

c_j	new solution at time j
c_jm1	old solution at time j-1
T_j	current/new value of time
T_jm1	previous value of time
X	distance along column
n	last index of distance array

Returns

void

Warning

{not tested, probably uses wrong value of n}

5.3 src/my_petsc.h File Reference

Functions and structs for solving PDE.

```
#include <stdbool.h>
#include <petsc.h>
#include "isotherm.h"
```

Include dependency graph for my_petsc.h:

Data Structures

- struct VecAndArray
- struct AppCtx

  Useful parameters for solving, Application context.
- struct Variables_j

  Analytical and numerical variables at time j (and jm1 if analytical)

Functions

- void print_user_params (AppCtx u)

  print user params associated with application
- PetscErrorCode InitializeVecAndArray (DM da, VecAndArray ∗x)

  Initialize Struct containing both vector and array.
- PetscErrorCode DestroyVecAndArray (DM da, VecAndArray ∗x)

  Destroy Struct containing both vector and array.
- PetscErrorCode one_time_step (SNES snes, DMDALocalInfo ∗p_info, AppCtx ∗p_user, Variables_j ∗p_vars)

  Perform one time step.
- PetscErrorCode simulate (DM da, SNES snes, DMDALocalInfo ∗p_info, AppCtx ∗p_user)

  Perform calculations at all time steps.
- PetscErrorCode run (int argc, char ∗∗args, int m, double eps, double tau_star, double theta, ISO ∗isotherm, bool compute_analytical, double ∗btc, bool make_movie, bool print_header)

  Main function called.
- PetscErrorCode UpdateAnalytical (DMDALocalInfo ∗info, PetscReal ∗c_j, PetscReal ∗c_jm1, AppCtx ∗user)

  Updates analytical solution.
- PetscErrorCode UpdateSolid (DMDALocalInfo ∗info, PetscReal ∗W_j, AppCtx ∗user)

  Update solid concentration.
- PetscErrorCode UpdateIsotherm (DMDALocalInfo ∗info, PetscReal ∗W, AppCtx ∗user)
- PetscReal eval_S_i_j (PetscReal f_j, PetscReal f_jm1, PetscReal exp_mdT, PetscReal S_jm1, PetscReal dT)

  evaluate value of solid concentration
- PetscReal eval_dS_i_j (PetscReal df_i_j, PetscReal dT)

  evaluates gradient in solid concentration wrt fluid

- PetscReal theta_rule (PetscReal val_i, PetscReal val_im1, PetscReal theta)

  does theta rule for discretization in space
- PetscErrorCode FormFunctionLocal (DMDALocalInfo ∗info, PetscReal ∗W_j, PetscReal ∗FF, AppCtx ∗user)

  residuals of nonlinear equations
- PetscErrorCode FormJacobianLocal (DMDALocalInfo ∗info, PetscReal ∗W_j, Mat J, Mat P, AppCtx ∗user)

  jacobian of nonlinear equations
- PetscErrorCode CalculateOmega (DMDALocalInfo ∗info, PetscReal ∗W, AppCtx ∗user)

  calculate ω

5.3.1 Detailed Description

Functions and structs for solving PDE.

Author

Robert F. DeJaco

5.3.2 Function Documentation

5.3.2.1 CalculateOmega()

```
PetscErrorCode CalculateOmega (
              DMDALocalInfo ∗ info,
              PetscReal ∗ W,
              AppCtx ∗ user )
```

calculate ω

Parameter used to determine if simulation is at steady state

Returns

void

Parameters

	info	grid object
in	*W*	solution
in,out	*user*	stores attribute omega

5.3.2.2 DestroyVecAndArray()

```
PetscErrorCode DestroyVecAndArray (
            DM da,
            VecAndArray * x )
```

Destroy Struct containing both vector and array.

See also

VecAndArray

Parameters

in	*da*	manages an abstract grid object and its interactions with the algebraic solvers
	x	Vector and array to destroy

5.3.2.3 eval_dS_i_j()

```
PetscReal eval_dS_i_j (
            PetscReal df_i_j,
            PetscReal dT )
```

evaluates gradient in solid concentration wrt fluid

returns gradient, $\Delta\tau F'/2/\varepsilon$

Parameters

in	*df_↩ i_j*	gradient in isotherm
in	*dT*	scaled time step, likely $\Delta\tau/\varepsilon$

5.3.2.4 eval_S_i_j()

```
PetscReal eval_S_i_j (
            PetscReal f_j,
            PetscReal f_jm1,
            PetscReal exp_mdT,
            PetscReal S_jm1,
            PetscReal dT )
```

evaluate value of solid concentration

Returns

value of solid concentration S_i^j

Parameters

f_j	value of adsorption isotherm at i and j
f_jm1	value of adsorption isotherm at i but j - 1
exp_mdT	value for $e^{-\Delta\tau/\varepsilon}$
S_jm1	Value for solid concentration at i but j - 1
dT	value for $\Delta\tau/\varepsilon$

5.3.2.5 FormFunctionLocal()

```
PetscErrorCode FormFunctionLocal (
             DMDALocalInfo * info,
             PetscReal * W_j,
             PetscReal * FF,
             AppCtx * user )
```

residuals of nonlinear equations

Returns

void

Parameters

info	Abstract object with grid info
W← _j	Solution, used to evaluate residuals
FF	residuals or form function
user	application context

5.3.2.6 FormJacobianLocal()

```
PetscErrorCode FormJacobianLocal (
             DMDALocalInfo * info,
             PetscReal * W_j,
             Mat J,
             Mat P,
             AppCtx * user )
```

jacobian of nonlinear equations

Returns

void

Parameters

info	Abstract object with grid info
W↩_j	Solution, used to evaluate residuals
J	not used?
P	jacobian
user	application context

5.3.2.7 InitializeVecAndArray()

```
PetscErrorCode InitializeVecAndArray (
            DM da,
            VecAndArray * x )
```

Initialize Struct containing both vector and array.

See also

VecAndArray

Parameters

in	*da*	manages an abstract grid object and its interactions with the algebraic solvers
	x	Vector and array to initialize

5.3.2.8 one_time_step()

```
PetscErrorCode one_time_step (
            SNES snes,
            DMDALocalInfo * p_info,
            AppCtx * p_user,
            Variables_j * p_vars )
```

Perform one time step.

Parameters

in	*snes*	Solver
in	*p_info*	Information about some parameters needed
in,out	*p_user*	Application context
out	*p_vars*	Variables at time j, updated for next time step

5.3.2.9 run()

```
PetscErrorCode run (
             int argc,
             char ** args,
             int m,
             double eps,
             double tau_star,
             double theta,
             ISO * isotherm,
             bool compute_analytical,
             double * btc,
             bool make_movie,
             bool print_header )
```

Main function called.

Parameters

in	*argc*	number of command arguments
in	*args*	command arguments
in	*m*	number of time steps
in	*eps*	value of epsilon ε
in	*tau_star*	total simulation time $\tau_\star$
in	*theta*	fraction of bfd/ffd
in	*isotherm*	adsorption isotherm struct. Needs to be allocated/initialized beforehand
in	*compute_analytical*	whether or not to compute analytical solution
in,out	*btc*	values of break-through curve
in	*make_movie*	whether or not to make movie
in	*print_header*	whether or not to print header

5.3.2.10 simulate()

```
PetscErrorCode simulate (
             DM da,
             SNES snes,
             DMDALocalInfo * p_info,
             AppCtx * p_user )
```

Perform calculations at all time steps.

Parameters

da	! Abstract grid object
snes	! solver
p_info	! local info on grid
p_user	User Application context

5.3.2.11 theta_rule()

```
PetscReal theta_rule (
            PetscReal val_i,
            PetscReal val_im1,
            PetscReal theta )
```

does theta rule for discretization in space

Returns

value of expression averaged wrt theta, $v_i(1-\theta)+v_{i-1}\theta$ for some v_i, v_{i-1}

Parameters

val_i	value at spatial index i
val_im1	value at spatial index i - 1
theta	value for $0 \leq \theta \leq 1$

5.3.2.12 UpdateAnalytical()

```
PetscErrorCode UpdateAnalytical (
            DMDALocalInfo * info,
            PetscReal * c_j,
            PetscReal * c_jm1,
            AppCtx * user )
```

Updates analytical solution.

Updates analytical solution for time j based off of info for $j-1$.

Parameters

`in`	*info*	information about local grid
`in,out`	*c_j*	new solution computed
`in`	*c_jm1*	old solution
`in`	*user*	Application context

5.3.2.13 UpdateIsotherm()

```
PetscErrorCode UpdateIsotherm (
            DMDALocalInfo * info,
            PetscReal * W,
            AppCtx * user )
```

Parameters

in	*info*	local information about grid
in	*W*	Solution of PDE at some value of time
in,out	*user*	application context. new values of isotherm stored here

5.3.2.14 UpdateSolid()

```
PetscErrorCode UpdateSolid (
            DMDALocalInfo * info,
            PetscReal * W_j,
            AppCtx * user )
```

Update solid concentration.

Parameters

in	*info*	information about grid
in	*W←↩ _j*	Numerical solution of fluid concentration
in	*user*	application context

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