XBraid Tutorial

A flexible and scalable approach to parallel-in-time

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Outline

1. Introduction
   → Tutorial software requirements and XBraid overview
2. Simplest example of solving a scalar ODE with `examples/ex-01`
   → Defining the `App` and `vector` structures, writing wrapper functions, running XBraid
3. Explore more XBraid settings in `examples/ex-01-expanded.c`
4. Porting a user-code to XBraid with `examples/ex-02`
   → Debugging the connection to XBraid
   → Intrusiveness versus efficiency
5. A few application area highlights

Appendix: *Advanced XBraid features*

- *Temporal adaptivity*
- *Shell-vectors and BDF-k*
- *Fortran90 Interface*
- *Residual and storage options*
- *Spatial coarsening*

To interact with the tutorial, you need

- This tutorial needs a working installation of XBraid 2.1 or higher
  `http://llnl.gov/casc/xbraid/`
  - See the User's manual for instructions on how to install XBraid
  - See the "Publications" page for a copy of this tutorial

XBraid v2.1 (or higher)	*required*
GCC compiler	*required*
MPI	*recommended*
Python 2.7 (or higher) with NumPy, Matplotlib	*recommended*
hypre installation for running ex-03 `http://llnl.gov/casc/hypre`	*optional*

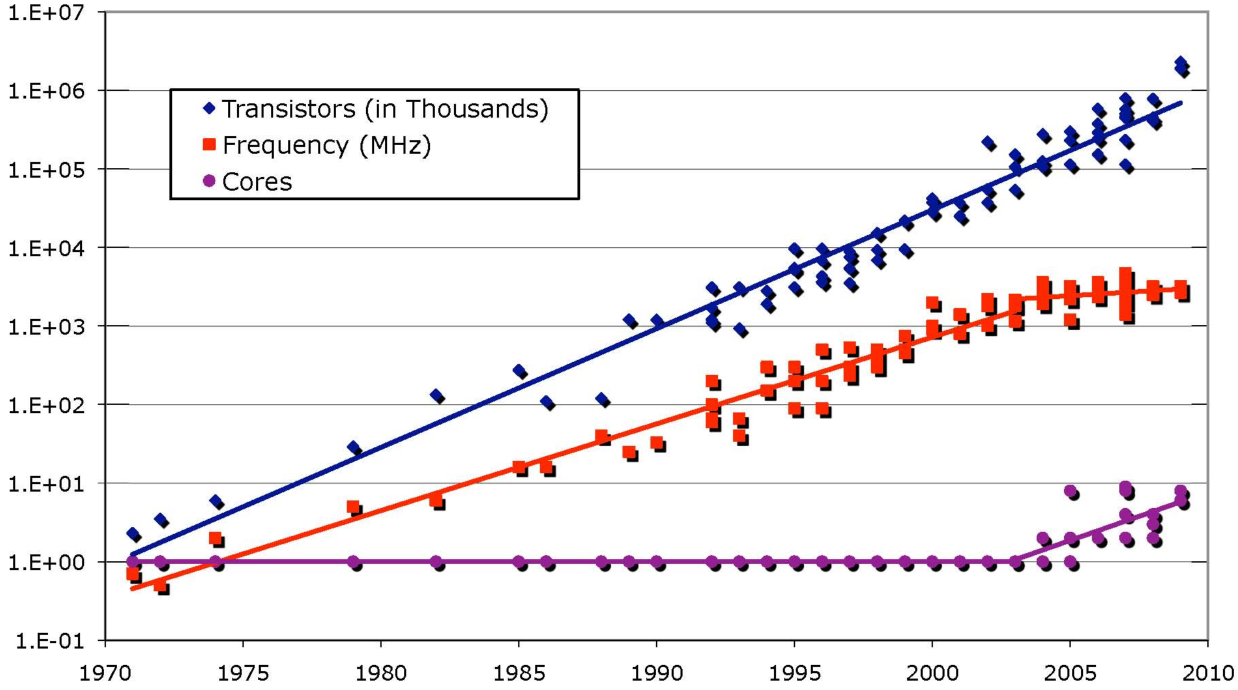
To interact with the tutorial, you need

- Make sure you can run

```
$ cd xbraid
$ make
$ cd examples
$ make ex-01 ex-02
$ ./ex-01
 Braid: || r_1 || = 2.845538e-02, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 8.621939e-04, conv factor = 3.03e-02, wall time = ...
 Braid: || r_3 || = 0.000000e+00, conv factor = 0.00e+00, wall time = ...
 ...
$ ./ex-02
 Braid: || r_0 || = 4.041694e+00, conv factor = 1.00e+00, wall time = ...
 Braid: || r_1 || = 1.037471e-01, conv factor = 2.57e-02, wall time = ...
 Braid: || r_2 || = 2.926906e-03, conv factor = 2.82e-02, wall time = ...
 ...
```

Traditional time integration will become a sequential bottleneck

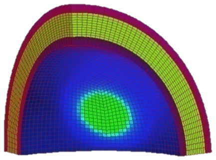
From Kathy Yelick's talk titled "Ten Ways to Waste a Parallel Computer."



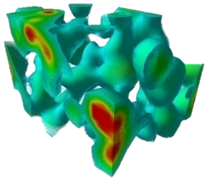
- Clock rates are no longer increasing – faster speed is now achieved through more concurrency
- Parallel time integration methods are needed (think exascale)!

Multigrid is well suited for exascale

- For many applications, the fastest and most scalable solvers are already multigrid methods



Elasticity / Plasticity



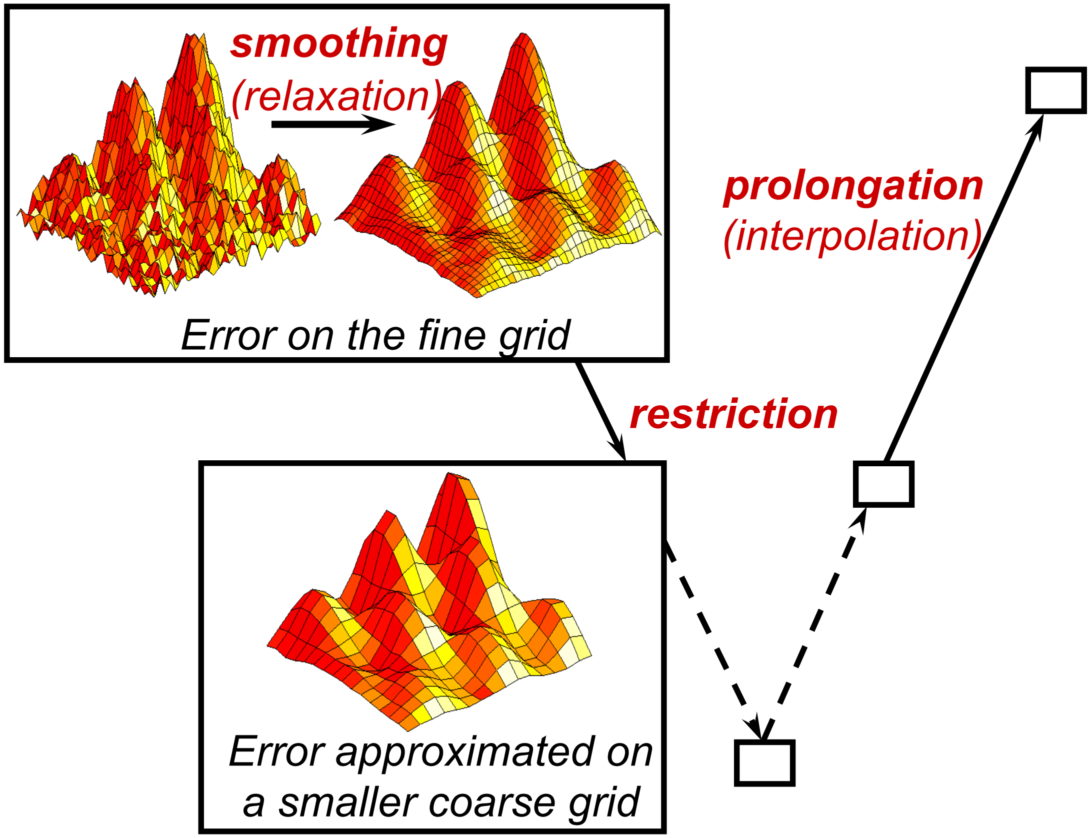
Quantum Chromodynamics

- Exascale solver algorithms will need to:
  - Exhibit extreme levels of parallelism (exascale → 1 billion cores)
    Spatial multigrid has already scaled to over 1 million cores
  - Minimize data movement
    Multigrid is $O(N)$ optimal
  - Exploit machine heterogeneity
    If the user's problem can exploit heterogenity, then so can multigrid
  - Be resilient to faults
    Multigrid has already shown good resilience (being iterative and multilevel helps)
- Apply multigrid to the temporal dimension!

Our approach for parallel-in-time

- Apply the wealth of research on parallel spatial multigrid to multigrid in time
- This is where our team has extensive experience (*hypre* project)

The Multigrid V-cycle



Technical approach

- Consider the **general** one-step method

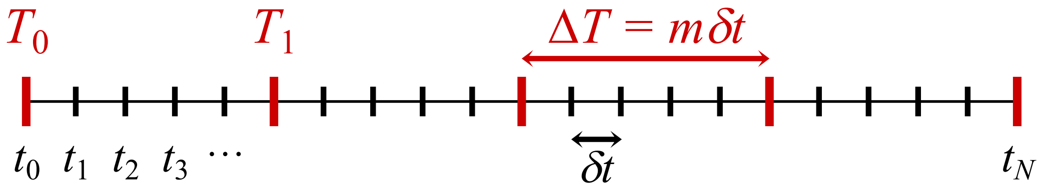
$$\boldsymbol{u}_i = \Phi_i(\boldsymbol{u}_{i-1}) + \boldsymbol{g}_i, \quad i = 1, 2, \ldots, N$$

- In the linear setting *(for simplicity)*, time marching $\equiv$ forward solve
  - This is an $O(N)$ direct method, **but sequential**

$$A\mathbf{u} \equiv \begin{pmatrix} I & & & \\ -\Phi & I & & \\ & \ddots & \ddots & \\ & & -\Phi & I \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \boldsymbol{u}_1 \\ \vdots \\ \boldsymbol{u}_N \end{pmatrix} = \begin{pmatrix} \boldsymbol{g}_0 \\ \boldsymbol{g}_1 \\ \vdots \\ \boldsymbol{g}_N \end{pmatrix} \equiv \mathbf{g}$$

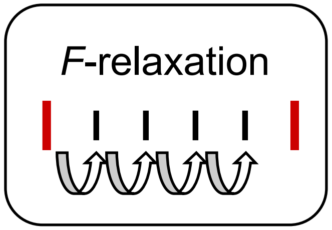
- We propose solving this system **iteratively** with a multigrid method
  - Extend multigrid reduction (MGR, 1979) to the time dimension
  - Coarsens only in time (non-intrusive)
  - $O(N)$, highly parallel

Technical approach



- F-point (fine grid only)
- C-point (coarse & fine grid)

- Relaxation is highly parallel
  - Alternates between F-points and C-points
  - F-point relaxation = integration over each coarse time interval



- Coarse system is a time rediscretization
  - Approximate impractical Φ^m with Φ_Δ a rediscretization with ΔT

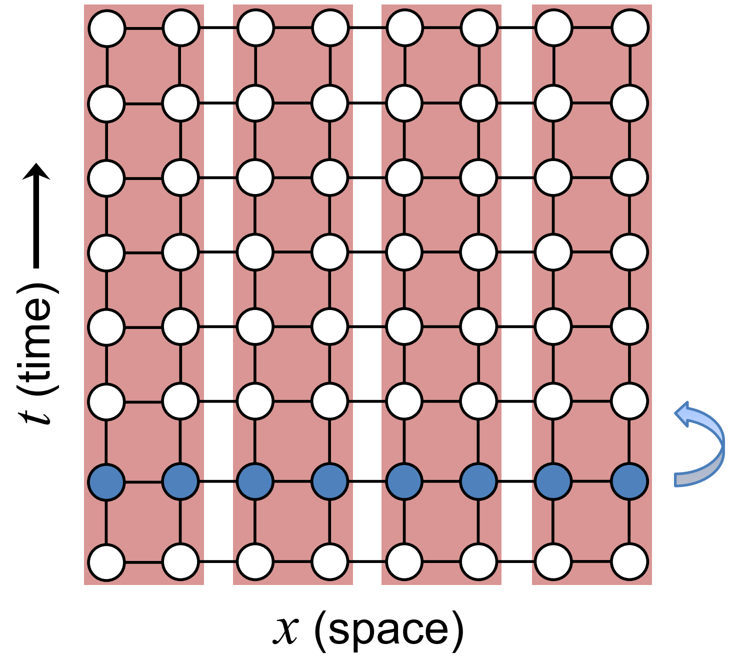
$$A_\Delta = \begin{pmatrix} I & & & \\ -\Phi^m & I & & \\ & \ddots & \ddots & \\ & & -\Phi^m & I \end{pmatrix} \quad \Rightarrow \quad A_\Delta = \begin{pmatrix} I & & & \\ -\Phi_\Delta & I & & \\ & \ddots & \ddots & \\ & & -\Phi_\Delta & I \end{pmatrix}$$

  - Apply recursively for multilevel hierarchy

Parallel decomposition

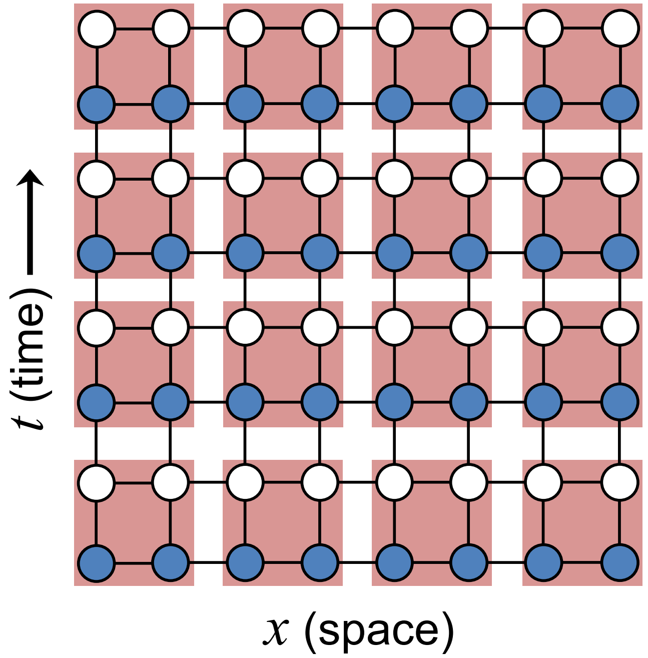
- Our code **XBraid** is agnostic to spatial decomposition and only parallelizes in time

Serial time stepping



Negative: Parallelize in space only
Positive: Store only one time step

Multigrid in time



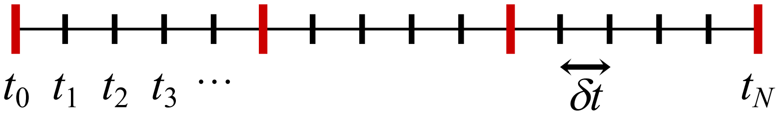
Positive: Parallelize in space and time
Negative: Store several time steps

Properties of the approach

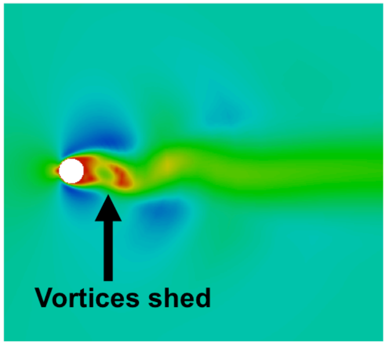
- Expose **concurrency** in the time dimension with multigrid
- **Non-intrusive**, with unchanged time discretization
- Converges to **same solution** as sequential time stepping

$$\begin{pmatrix} I & & & \\ -\Phi & I & & \\ & \ddots & \ddots & \\ & & -\Phi & I \end{pmatrix}$$

- Only store C-points to minimize storage
- Optimal for variety of parabolic problems
  - Converges in ~10 iterations for any coarsening factor
  - Larger factors require larger (sequential) F-relaxation intervals



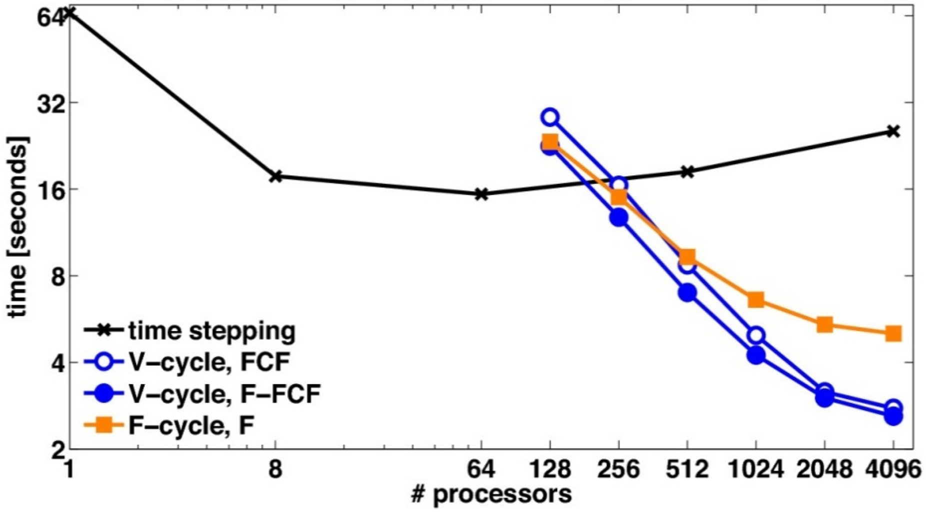
- Extends to **nonlinear** problems with FAS formulation
- In simple two-level setting, our method is **equivalent to parareal**
  - This is a popular method, typically not viewed as multigrid



- Many active research topics
  - Adaptivity in time, moving meshes and multistep methods all possible
  - Space-time coarsening possible (stability on coarse time-grids for explicit schemes)

Huge parallel speedups available, but in a new way

- Time stepping is already $O(N)$
- Useful only beyond a crossover
- Need 10-100x more parallelism just to break even

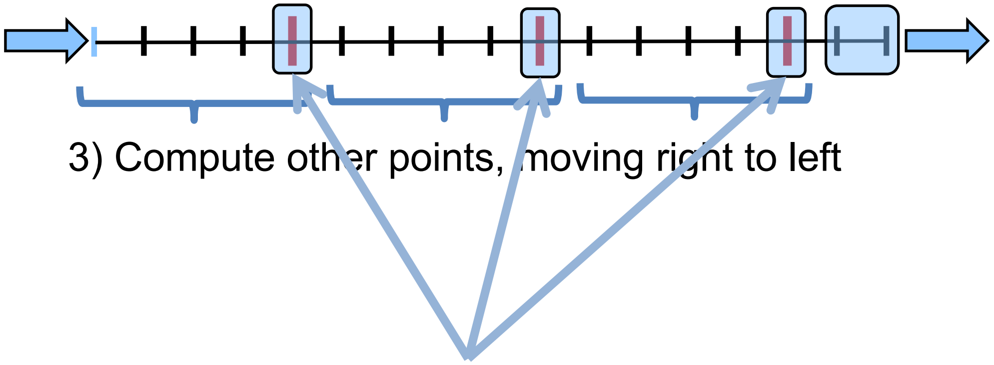


3D Heat Equation: 33^3 x 4097,
8 procs in space, 6x speedup

- The more time steps, the more speedup potential
  - Applications that require lots of time steps will benefit first
  - Speedups (so far) up to 52x on 100K total cores

XBraid: open source, non-intrusive and flexible

- Overlap communication and computation
  - Consider relaxation over a processor's portion of the time interval
  - Start computation with right-most interval to overlap comm/comp



1) Post receive

2) Compute and send

3) Compute other points, moving right to left

- Code stores only C-points to minimize storage
  - Ability to coarsen by large factors means fewer parallel resources
  - Memory multiplier per processor
    ~$O(\log N)$ with time coarsening, $O(1)$ with space-time coarsening

XBraid: open source, non-intrusive and flexible

- User defines two objects:
  - `App` and `Vector`
- User also writes several wrapper routines:
  - *`Step, Init, Clone, Sum, SpatialNorm, Access, BufPack, BufUnpack, BufSize`*
  - For optional spatial coarsening: `Coarsen, Refine`
- Example: `Step(app, u, status)`
  - Advances vector u from time `tstart` to `tstop`
  - Returns a target refinement factor

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Appendix: *Advanced XBraid features*

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Simplest Example: Scalar ODE

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- First, you must define your `app` and `vector` structures

This is your simulation application structure. Place any time-independent data here, which is needed to take a time step.

Here, we only need the MPI rank in the App structure (for later file output).

```
typedef struct _braid_App_struct{
   int       rank;
} my_App;


typedef struct _braid_Vector_struct{
   double value;
} my_Vector;
```

Simplest Example: Scalar ODE

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- First, you must define your `app` and `vector` structures

This is your state vector structure. It holds any time-dependent information that should stay with a vector, e.g. mesh information and unknowns.

For this problem, the vector is one double.

```
typedef struct _braid_App_struct{
   int         rank;
} my_App;


typedef struct _braid_Vector_struct{
   double value;
} my_Vector;
```

Define the `Step()` function

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$

`Step()` evolves `u` from `tstart` to `tstop`

```
int my_Step(braid_App          app,
            braid_Vector       ustop,
            braid_Vector       fstop,
            braid_Vector       u,
            braid_StepStatus status)
{
   double tstart;
   double tstop;
   braid_StepStatusGetTstartTstop(status, &tstart, &tstop);

   (u->value) = 1./(1. + tstop-tstart)*(u->value);

   return 0;
}
```

Define the `Step()` function

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$

The `app` structure is passed into every user-written function.

```
int my_Step(braid_App         app,
            braid_Vector      ustop,
            braid_Vector      fstop,
            braid_Vector      u,
            braid_StepStatus  status)
{
   double tstart;
   double tstop;
   braid_StepStatusGetTstartTstop(status, &tstart, &tstop);

   (u->value) = 1./(1. + tstop-tstart)*(u->value);

   return 0;
}
```

Define the `Step()` function

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$

Vector at `tstop` from previous XBraid iteration (initial guess for implicit solvers)

```
int my_Step(braid_App        app,
            braid_Vector     ustop,
            braid_Vector     fstop,
            braid_Vector     u,
            braid_StepStatus status)
{
   double tstart;
   double tstop;
   braid_StepStatusGetTstartTstop(status, &tstart, &tstop);

   (u->value) = 1./(1. + tstop-tstart)*(u->value);

   return 0;
}
```

Define the `Step()` function

- File: `examples/ex-01.c`   Solves: $u_t = \lambda u$

Vector at `tstart`

```
int my_Step(braid_App          app,
            braid_Vector       ustop,
            braid_Vector       fstop,
            braid_Vector       u,
            braid_StepStatus   status)
{
   double tstart;
   double tstop;
   braid_StepStatusGetTstartTstop(status, &tstart, &tstop);

   (u->value) = 1./(1. + tstop-tstart)*(u->value);

   return 0;
}
```

Define the `Step()` function

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$

Ignore by default. (XBraid forcing term, only needed if residual option is used)

```
int my_Step(braid_App        app,
            braid_Vector     ustop,
            braid_Vector     fstop,
            braid_Vector     u,
            braid_StepStatus status)
{
   double tstart;
   double tstop;
   braid_StepStatusGetTstartTstop(status, &tstart, &tstop);

   (u->value) = 1./(1. + tstop-tstart)*(u->value);

   return 0;
}
```

Define the `Step()` function

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$

Status structures can be queried for various information (level, iteration, etc...)

```
int my_Step(braid_App         app,
            braid_Vector      ustop,
            braid_Vector      fstop,
            braid_Vector      u,
            braid_StepStatus  status)
{
   double tstart;
   double tstop;
   braid_StepStatusGetTstartTstop(status, &tstart, &tstop);

   (u->value) = 1./(1. + tstop-tstart)*(u->value);

   return 0;
}
```

Define the `Step()` function

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$

For instance, to get `tstart, tstop`

```
int my_Step(braid_App          app,
            braid_Vector       ustop,
            braid_Vector       fstop,
            braid_Vector       u,
            braid_StepStatus status)
{
   double tstart;
   double tstop;
   braid_StepStatusGetTstartTstop(status, &tstart, &tstop);

   (u->value) = 1./(1. + tstop-tstart)*(u->value);

   return 0;
}
```

Define the `Step()` function

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$

Take backward Euler step

```
int my_Step(braid_App          app,
            braid_Vector       ustop,
            braid_Vector       fstop,
            braid_Vector       u,
            braid_StepStatus status)
{
   double tstart;
   double tstop;
   braid_StepStatusGetTstartTstop(status, &tstart, &tstop);

   (u->value) = 1./(1. + tstop-tstart)*(u->value);

   return 0;
}
```

Define other wrapper functions

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- Define functions: `Init`, `Clone`, `Free`, **`Sum`**, `SpatialNorm`, `Access`, `BufPack`, `BufUnpack`,`BufSize`

Again, we see the app structure being passed in

```
int my_Sum(braid_App      app,
           double         alpha,
           braid_Vector   x,
           double         beta,
           braid_Vector   y)
{
   (y->value) = alpha*(x->value) + beta*(y->value);
   return 0;
}
```

Define other wrapper functions

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- Define functions: `Init`, `Clone`, `Free`, **`Sum`**, `SpatialNorm`, `Access`, `BufPack`, `BufUnpack`, `BufSize`

This function carries out a simple AXPY operation

```
int my_Sum(braid_App      app,
           double         alpha,
           braid_Vector   x,
           double         beta,
           braid_Vector   y)
{
   (y->value) = alpha*(x->value) + beta*(y->value);
   return 0;
}
```

Define other wrapper functions

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- Define functions: `Init`, `Clone`, `Free`, `Sum`, `SpatialNorm`, **`Access`**, `BufPack`, `BufUnpack`, `BufSize`

This function is how the user accesses the solution

- **By default, it is called at the end of the simulation for every time point**
- **Using `braid_AccessSetLevel()` allows for more frequent access**

```
int my_Access(braid_App          app,
              braid_Vector       u,
              braid_AccessStatus astatus)
{
   int  index;  char  filename[255];  FILE  *file;

   braid_AccessStatusGetTIndex(astatus, &index);
   sprintf(filename, "%s.%04d.%03d", "ex-01.out", index, app->rank);
   file = fopen(filename, "w");
   fprintf(file, "%.14e\n", (u->value));

   fflush(file);  fclose(file); return 0;
}
```

Define other wrapper functions

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- Define functions: `Init`, `Clone`, `Free`, `Sum`, `SpatialNorm`, **`Access`**, `BufPack`, `BufUnpack`,`BufSize`

Here, we just write a single solution value to individual files

```
int my_Access(braid_App          app,
              braid_Vector       u,
              braid_AccessStatus astatus)
{
   int  index;  char  filename[255];  FILE  *file;

   braid_AccessStatusGetTIndex(astatus, &index);
   sprintf(filename, "%s.%04d.%03d", "ex-01.out", index, app->rank);
   file = fopen(filename, "w");
   fprintf(file, "%.14e\n", (u->value));

   fflush(file);  fclose(file); return 0;
}
```

Define other wrapper functions

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- Define functions: `Init, Clone, Free, Sum, SpatialNorm, Access,` **`BufPack`**`, BufUnpack,BufSize`

The `Buf*` functions tell XBraid how to pack, unpack and size MPI Buffers

Define other wrapper functions

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- Define functions: `Init, Clone, Free, Sum, SpatialNorm, Access,` **`BufPack`**`, BufUnpack,BufSize`

`BufPack()` flattens the vector `u` into `buffer`

```
int my_BufPack(braid_App             app,
               braid_Vector          u,
               void                 *buffer,
               braid_BufferStatus bstatus)
{
   double *dbuffer = buffer;

   dbuffer[0] = (u->value);
   braid_BufferStatusSetSize( bstatus, sizeof(double) );

   return 0;
}
```

Define other wrapper functions

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- Define functions: `Init`, `Clone`, `Free`, `Sum`, `SpatialNorm`, `Access`, **`BufPack`**, `BufUnpack`,`BufSize`

Packing this buffer entails just setting a single double value

```
int my_BufPack(braid_App            app,
               braid_Vector         u,
               void                 *buffer,
               braid_BufferStatus bstatus)
{
   double *dbuffer = buffer;

   dbuffer[0] = (u->value);
   braid_BufferStatusSetSize( bstatus, sizeof(double) );

   return 0;
}
```

Define other wrapper functions

- File: `examples/ex-01.c`   Solves: $u_t = \lambda u$
- Define functions: `Init`, `Clone`, `Free`, `Sum`, `SpatialNorm`, `Access`, **`BufPack`**, `BufUnpack`,`BufSize`

This is an example of returning a value (the buffer size) with a status structure

```
int my_BufPack(braid_App           app,
               braid_Vector        u,
               void                *buffer,
               braid_BufferStatus bstatus)
{
   double *dbuffer = buffer;

   dbuffer[0] = (u->value);
   braid_BufferStatusSetSize( bstatus, sizeof(double) );

   return 0;
}
```

Initialize App and XBraid

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- The next step is to setup XBraid in `main()`

```
int main()
   ...
   braid_Core    core;
   ntime  = 10;
   tstart = 0.0; tstop  = 5.0;
   ...
   app = (my_App *) malloc(sizeof(my_App));
   app->rank)    = rank;
   ...
   braid_Init(MPI_COMM_WORLD, MPI_COMM_WORLD, tstart, tstop,
              ntime, app, my_Step, my_Init, my_Clone,
              my_Free, my_Sum, my_SpatialNorm,
              my_Access, my_BufSize, my_BufPack,
              my_BufUnpack, &core);
```

Initialize App and XBraid

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- The next step is to setup XBraid in `main()`

`braid_Core` is the core data structure, holding all of XBraid’s internals

```
int main()
  ...
  braid_Core    core;
  ntime  = 10;
  tstart = 0.0; tstop  = 5.0;
  ...
  app = (my_App *) malloc(sizeof(my_App));
  (app->rank)   = rank;
  ...
  braid_Init(MPI_COMM_WORLD, MPI_COMM_WORLD, tstart, tstop,
             ntime, app, my_Step, my_Init, my_Clone,
             my_Free, my_Sum, my_SpatialNorm,
             my_Access, my_BufSize, my_BufPack,
             my_BufUnpack, &core);
```

Initialize App and XBraid

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- The next step is to setup XBraid in `main()`

Define your time domain

```
int main()
   ...
   braid_Core    core;
   ntime  = 10;
   tstart = 0.0; tstop  = 5.0;
   ...
   app = (my_App *) malloc(sizeof(my_App));
   (app->rank)    = rank;
   ...
   braid_Init(MPI_COMM_WORLD, MPI_COMM_WORLD, tstart, tstop,
              ntime, app, my_Step, my_Init, my_Clone,
              my_Free, my_Sum, my_SpatialNorm,
              my_Access, my_BufSize, my_BufPack,
              my_BufUnpack, &core);
```

Initialize App and XBraid

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- The next step is to setup XBraid in `main()`

Initialize `App` structure

```
int main()
   ...
   braid_Core    core;
   ntime  = 10;
   tstart = 0.0; tstop  = 5.0;
   ...
   app = (my_App *) malloc(sizeof(my_App));
   (app->rank)    = rank;
   ...
   braid_Init(MPI_COMM_WORLD, MPI_COMM_WORLD, tstart, tstop,
              ntime, app, my_Step, my_Init, my_Clone,
              my_Free, my_Sum, my_SpatialNorm,
              my_Access, my_BufSize, my_BufPack,
              my_BufUnpack, &core);
```

Initialize App and XBraid

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- The next step is to setup XBraid in `main()`

Initialize `braid_Core`, passing in all user-written functions

```
int main()
   ...
   braid_Core    core;
   ntime  = 10;
   tstart = 0.0; tstop  = 5.0;
   ...
   app = (my_App *) malloc(sizeof(my_App));
   (app->rank)    = rank;
   ...
   braid_Init(MPI_COMM_WORLD, MPI_COMM_WORLD, tstart, tstop,
              ntime, app, my_Step, my_Init, my_Clone,
              my_Free, my_Sum, my_SpatialNorm,
              my_Access, my_BufSize, my_BufPack,
              my_BufUnpack, &core);
```

Set XBraid options and run

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- The next step is to setup XBraid in `main()`

Set all the XBraid options that you want

```
int main()
   ...
   braid_SetPrintLevel( core, 1);
   braid_SetMaxLevels(core, 2);
   braid_SetAbsTol(core, 1.0e-06);
   braid_SetCFactor(core, -1, 2);

   braid_Drive(core);

   braid_Destroy(core);
```

Set XBraid options and run

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- The next step is to setup XBraid in `main()`

Run the simulation

```
int main()
  ...
  braid_SetPrintLevel( core, 1);
  braid_SetMaxLevels(core, 2);
  braid_SetAbsTol(core, 1.0e-06);
  braid_SetCFactor(core, -1, 2);

  braid_Drive(core);

  braid_Destroy(core);
```

Set XBraid options and run

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- The next step is to setup XBraid in `main()`

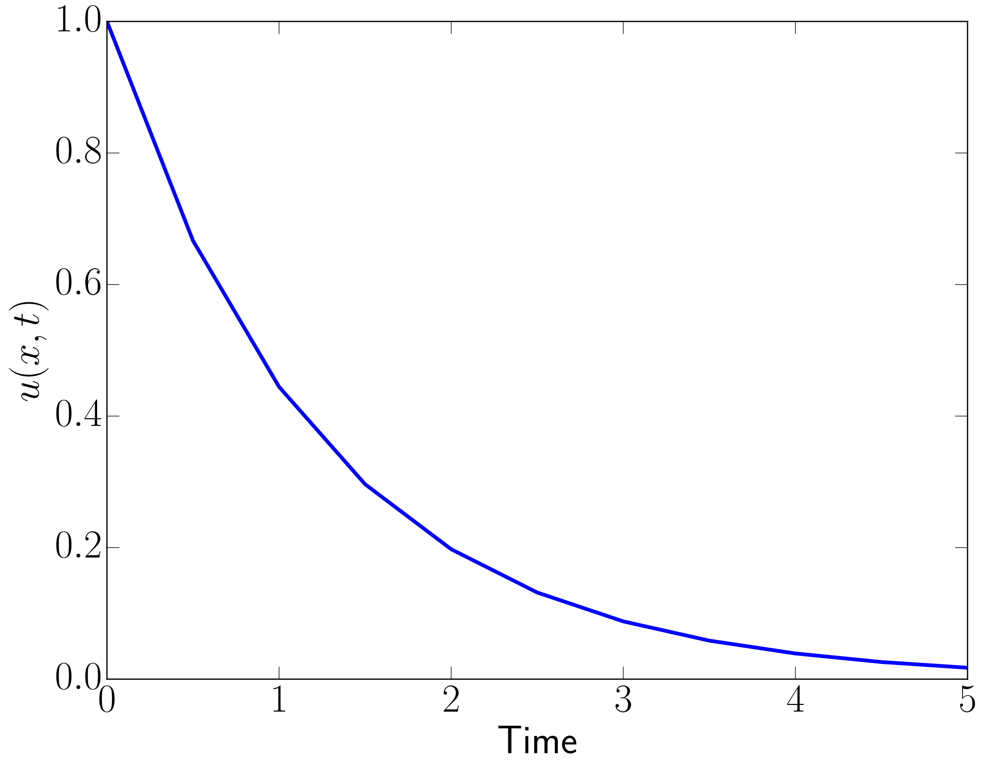
Clean up

```
int main()
   ...
   braid_SetPrintLevel( core, 1);
   braid_SetMaxLevels(core, 2);
   braid_SetAbsTol(core, 1.0e-06);
   braid_SetCFactor(core, -1, 2);

   braid_Drive(core);

   braid_Destroy(core);
```

Output

- File: `examples/ex-01.c` Solves: $u_t = \lambda u$
- Finally! We can run the example.

```
$ cd examples
$ make ex-01
$ ./ex-01
$ cat ex-01.out.00*
  1.00000000000000e+00
  6.66666666666667e-01
  4.44444444444444e-01
  2.96296296296296e-01
  1.97530864197531e-01
  1.31687242798354e-01
  8.77914951989026e-02
  5.85276634659351e-02
  3.90184423106234e-02
  2.60122948737489e-02
  1.73415299158326e-02
```



Outline

1. Introduction
   → Tutorial software requirements and XBraid overview
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   → Defining the `App` and `vector` structures, writing wrapper functions, running XBraid
3. Explore more XBraid settings in `examples/ex-01-expanded.c`
4. Porting a user-code to XBraid with `examples/ex-02`
   → Debugging the connection to XBraid
   → Intrusiveness versus efficiency
5. A few application area highlights

Appendix: *Advanced XBraid features*

- *Temporal adaptivity*
- *Shell-vectors and BDF-k*
- *Fortran90 Interface*
- *Residual and storage options*
- *Spatial coarsening*

Moving to `ex-01-expanded.c`

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$
- Adds more XBraid features and a command line interface to `ex-01.c`

Let’s experiment with these options!

```
$ cd examples
$ make ex-01-expanded
$ ./ex-01-expanded -help

-ntime <ntime>     : set num time points
-ml   <max_levels> : set max levels
-nu   <nrelax>     : set num F-C relaxations
-nu0  <nrelax>     : set num F-C relaxations on level 0
-tol  <tol>        : set stopping tolerance
-cf   <cfactor>    : set coarsening factor
-mi   <max_iter>   : set max iterations
-fmg               : use FMG cycling
-res               : use my residual
-tg <mydt>         : use user-specified time grid
                     1 - uniform time grid
                     2 - nonuniform time grid
```

Examine the standard XBraid output

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Residual history is printed out, along with convergence factors and wall times

```
$ ./ex-01-expanded
 Braid: Begin simulation, 10 time steps
 Braid: || r_0 || not available, wall time = 1.81e-04
 Braid: || r_1 || = 2.845538e-02, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 8.621939e-04, conv factor = 3.03e-02, wall time = ...
 Braid: || r_3 || = 0.000000e+00, conv factor = 0.00e+00, wall time = ...

 start time = 0.000000e+00
 stop time  = 5.000000e+00
 time steps = 10

 use seq soln?         = 0
 storage               = -1

 stopping tolerance    = 1.000000e-06
 use relative tol?     = 0
 max iterations        = 100
 iterations            = 4
 residual norm         = 0.000000e+00
                         --> 2-norm TemporalNorm
```

Examine the standard XBraid output

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Basic time domain information

```
$ ./ex-01-expanded
 Braid: Begin simulation, 10 time steps
 Braid: || r_0 || not available, wall time = 1.81e-04
 Braid: || r_1 || = 2.845538e-02, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 8.621939e-04, conv factor = 3.03e-02, wall time = ...
 Braid: || r_3 || = 0.000000e+00, conv factor = 0.00e+00, wall time = ...

 start time = 0.000000e+00
 stop time  = 5.000000e+00
 time steps = 10

 use seq soln?          = 0
 storage                = -1

 stopping tolerance     = 1.000000e-06
 use relative tol?      = 0
 max iterations         = 100
 iterations             = 4
 residual norm          = 0.000000e+00
                          --> 2-norm TemporalNorm
```

Examine the standard XBraid output

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Advanced options

```
$ ./ex-01-expanded
 Braid: Begin simulation, 10 time steps
 Braid: || r_0 || not available, wall time = 1.81e-04
 Braid: || r_1 || = 2.845538e-02, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 8.621939e-04, conv factor = 3.03e-02, wall time = ...
 Braid: || r_3 || = 0.000000e+00, conv factor = 0.00e+00, wall time = ...

 start time = 0.000000e+00
 stop time  = 5.000000e+00
 time steps = 10

 use seq soln?         = 0
 storage               = -1

 stopping tolerance    = 1.000000e-06
 use relative tol?     = 0
 max iterations        = 100
 iterations            = 4
 residual norm         = 0.000000e+00
                         --> 2-norm TemporalNorm
```

Examine the standard XBraid output

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Describe the XBraid options set for this run

```
$ ./ex-01-expanded
 Braid: Begin simulation, 10 time steps
 Braid: || r_0 || not available, wall time = ...
 Braid: || r_1 || = 2.845538e-02, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 8.621939e-04, conv factor = 3.03e-02, wall time = ...
 Braid: || r_3 || = 0.000000e+00, conv factor = 0.00e+00, wall time = ...

 start time = 0.000000e+00
 stop time  = 5.000000e+00
 time steps = 10

 use seq soln?         = 0
 storage               = -1

 stopping tolerance    = 1.000000e-06
 use relative tol?     = 0
 max iterations        = 100
 iterations            = 4
 residual norm         = 0.000000e+00
                         --> 2-norm TemporalNorm
```

Examine the standard XBraid output

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Describe the XBraid options set for this run

```
$ ./ex-01-expanded
 Braid: Begin simulation, 10 time steps
 ...

 use fmg?              = 0
 access_level          = 1
 print_level           = 1

 max number of levels  = 2
 min coarse            = 2
 number of levels      = 2
 skip down cycle       = 1
 number of refinements = 0

 level   time-pts   cfactor   nrelax
      0        10        2        1
      1         5

 wall time = ...
```

Examine the standard XBraid output

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Describes the levels in the XBraid hierarchy

```
$ ./ex-01-expanded
 Braid: Begin simulation, 10 time steps
 ...

 use fmg?               = 0
 access_level           = 1
 print_level            = 1

 max number of levels   = 2
 min coarse             = 2
 number of levels       = 2
 skip down cycle        = 1
 number of refinements  = 0

 level   time-pts   cfactor   nrelax
     0         10         2        1
     1          5

 wall time = ...
```

Increase number of time points

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Now, compare the effects of increasing the time domain size

```
$ ./ex-01-expanded -ntime 16
 Braid: Begin simulation, 16 time steps
 Braid: || r_0 || not available, wall time = …
 Braid: || r_1 || = 2.851025e-02, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 1.040035e-03, conv factor = 3.65e-02, wall time = ...
 Braid: || r_3 || = 3.530338e-05, conv factor = 3.39e-02, wall time = ...
 Braid: || r_4 || = 3.716892e-07, conv factor = 1.05e-02, wall time = ...
 ...

$ ./ex-01-expanded -ntime 128
 Braid: Begin simulation, 128 time steps
 Braid: || r_0 || not available, wall time = ...
 Braid: || r_1 || = 2.851112e-02, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 1.049429e-03, conv factor = 3.68e-02, wall time = ...
 Braid: || r_3 || = 4.437913e-05, conv factor = 4.23e-02, wall time = ...
 Braid: || r_4 || = 1.990483e-06, conv factor = 4.49e-02, wall time = ...
 Braid: || r_5 || = 9.174722e-08, conv factor = 4.61e-02, wall time = ...
 ...
```

FCF-relaxation

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Observe how changing the number of FCF-relaxations improves convergence

```
 $ ./ex-01-expanded -ntime 128 -nu 0
  Braid: Begin simulation, 128 time steps
  Braid: || r_0 || not available, wall time = ...
  Braid: || r_1 || = 6.415003e-02, conv factor = 1.00e+00, wall time = ...
  Braid: || r_2 || = 5.312734e-03, conv factor = 8.28e-02, wall time = ...
  Braid: || r_3 || = 5.055060e-04, conv factor = 9.51e-02, wall time = ...
  Braid: || r_4 || = 5.101391e-05, conv factor = 1.01e-01, wall time = ...
  Braid: || r_5 || = 5.290607e-06, conv factor = 1.04e-01, wall time = ...
  Braid: || r_6 || = 5.570496e-07, conv factor = 1.05e-01, wall time = ...

 $ ./ex-01-expanded -ntime 128 -nu 3
  Braid: Begin simulation, 128 time steps
  Braid: || r_0 || not available, wall time = ...
  Braid: || r_1 || = 5.631827e-03, conv factor = 1.00e+00, wall time = ...
  Braid: || r_2 || = 4.094709e-05, conv factor = 7.27e-03, wall time = ...
  Braid: || r_3 || = 3.420453e-07, conv factor = 8.35e-03, wall time = ...
```

Halting tolerance and max-iterations

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Observe how changing the tolerance and max-iter (-mi) parameters affect XBraid

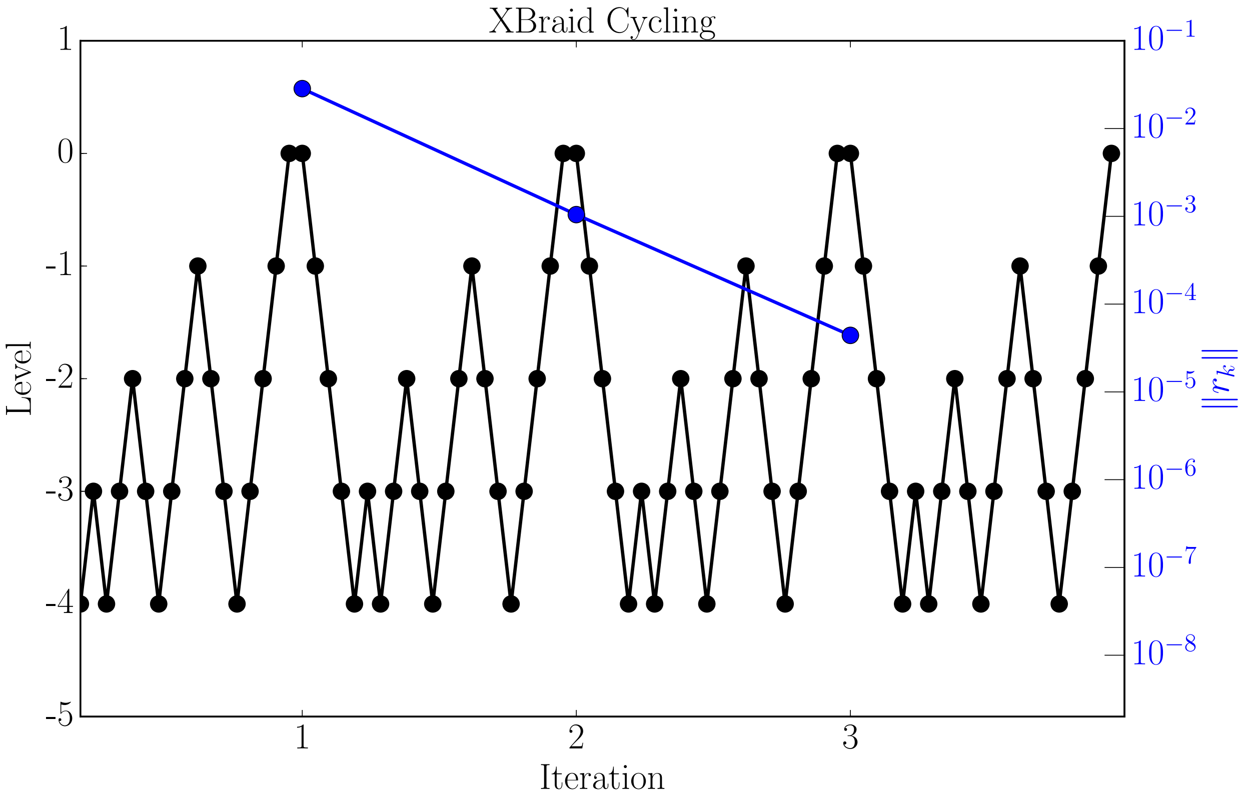
```
$./ex-01-expanded -ntime 128 -tol 1e-3
...
iterations                     = 4
...

$./ex-01-expanded -ntime 128 -tol 1e-12
...
iterations                     = 10
...

$./ex-01-expanded -ntime 128 -tol 1e-12 -mi 3
...
iterations                     = 3
...
```

Full multigrid cycles (FMG)

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Now, use the fmg parameter and plot braid.out.cycle (file generated at runtime)

```
$ ./ex-01-expanded -ntime 32 -ml 15 -mi 4 -fmg
$ python ../user_utils/cycleplot.py
```



This functionality can be used to adaptively refine in time (nested iteration)

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How to convert a user-code

- File: `examples/ex-02*`

Solves: $u_t = -u_{xx}$

ex-02-serial.c

```
/* Set up simulation */
t= 0.0; tstop= 2*PI; ...

/* Initialize u(t=0) */
get_solution(values, ...);


/* Loop over all time values */
for(step=1; step < ntime; step++){
   t = t + deltaT;
   take_step(values, t, ...);
}


/* Process result */
compute_error_norm(values, ...);
save_solution(fname, values, ...);
```

```
$ex-02-serial -ntime 64 -nspace 17
```

ex-02-lib.c

```
/* Common functions with XBraid */

/* Initialization routine */
void get_solution(...)

/* Helpers for take_step */
void solve_tridiag(...)
void matvec_tridiag(...)
void compute_stencil(...)

/* Core time-stepping routine */
void take_step(...)

/* Output Functions */
double compute_error_norm(...)
void save_solution(...)

/* XBraid specific spatial
interpolation/coarsening */
void interpolate_1D(...)
void coarsen_1D(...)
```

ex-02.c

```
XBraid
Driver
 ...
```

How to convert a user-code

- File: `examples/ex-02*` Solves: $u_t = -u_{xx}$

ex-02-serial.c

```
/* Set up simulation */
t= 0.0; tstop= 2*PI; ...

/* Initialize u(t=0) */
get_solution(values, ...);


/* Loop over all time values */
for(step=1; step < ntime; step++){
   t = t + deltaT;
   take_step(values, t, ...);
}


/* Process result */
compute_error_norm(values, ...);
save_solution(fname, values, ...);
```

```
$ex-02-serial -ntime 64 -nspace 17
```

ex-02-lib.c

```
/* Common functions with XBraid */

/* Initialization routine */
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/* Helpers for take_step */
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void matvec_tridiag(...)
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void interpolate_1D(...)
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```

ex-02.c

```
XBraid
Driver
...
```

How to convert a user-code

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Solves: $u_t = -u_{xx}$

ex-02-serial.c

```
/* Set up simulation */
t= 0.0; tstop= 2*PI; ...

/* Initialize u(t=0) */
get_solution(values, ...);


/* Loop over all time values */
for(step=1; step < ntime; step++){
   t = t + deltaT;
   take_step(values, t, ...);
}


/* Process result */
compute_error_norm(values, ...);
save_solution(fname, values, ...);
```

```
$ex-02-serial -ntime 64 -nspace 17
```

ex-02-lib.c

```
/* Common functions with XBraid */

/* Initialization routine */
void get_solution(...)

/* Helpers for take_step */
void solve_tridiag(...)
void matvec_tridiag(...)
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void interpolate_1D(...)
void coarsen_1D(...)
```

ex-02.c

```
XBraid
Driver
...
```

How to convert a user-code

- File: `examples/ex-02*`

Solves: $u_t = -u_{xx}$

ex-serial.c

```
Serial
Driver
 ...
```

ex-02-lib.c

```
/* Common functions with XBraid */

/* Initialization routine */
void get_solution(...)

/* Helpers for take_step */
void solve_tridiag(...)
void matvec_tridiag(...)
void compute_stencil(...)

/* Core time-stepping routine */
void take_step(...)

/* Output Functions */
double compute_error_norm(...)
void save_solution(...)

/* XBraid specific spatial
interpolation/coarsening */
void interpolate_1D(...)
void coarsen_1D(...)
```

ex-02.c

```
typedef struct _braid_App_struct
 MPI_Comm   comm;
 double     matrix[3];
 ...

typedef struct _braid_Vector_struct
 int      size;
 double *values;

int my_Step(u, ...)
 take_step(u->values, ...);

int my_Access(u, ...)
 compute_error_norm(u->values, ...);
 save_solution(fname, u->values, ...);

int my_Init(u, ...)
 get_solution(u->values, ...);

main()
 braid_Core core; app = (my_App *) ...
 braid_Init(..., core);
 braid_Drive(core);
```

App structure holds time-independent data for stepping

How to convert a user-code

- File: `examples/ex-02*` Solves: $u_t = -u_{xx}$

ex-serial.c

```
Serial
Driver
...
```

ex-02-lib.c

```
/* Common functions with XBraid */

/* Initialization routine */
void get_solution(...)

/* Helpers for take_step */
void solve_tridiag(...)
void matvec_tridiag(...)
void compute_stencil(...)

/* Core time-stepping routine */
void take_step(...)

/* Output Functions */
double compute_error_norm(...)
void save_solution(...)

/* XBraid specific spatial
interpolation/coarsening */
void interpolate_1D(...)
void coarsen_1D(...)
```

ex-02.c

```
typedef struct _braid_App_struct
 MPI_Comm  comm;
 double    matrix[3];
 ...

typedef struct _braid_Vector_struct
 int     size;
 double *values;

int my_Step(u, ...)
 take_step(u->values, ...);

int my_Access(u, ...)
 compute_error_norm(u->values, ...);
 save_solution(fname, u->values, ...);

int my_Init(u, ...)
 get_solution(u->values, ...);

main()
 braid_Core core; app = (my_App *) ...
 braid_Init(..., core);
 braid_Drive(core);
```

Vector holds time-dependent data for stepping

How to convert a user-code

- File: `examples/ex-02*` Solves: $u_t = -u_{xx}$

ex-serial.c

```
Serial
Driver
 ...
```

ex-02-lib.c

```
/* Common functions with XBraid */

/* Initialization routine */
void get_solution(...)

/* Helpers for take_step */
void solve_tridiag(...)
void matvec_tridiag(...)
void compute_stencil(...)

/* Core time-stepping routine */
void take_step(...)

/* Output Functions */
double compute_error_norm(...)
void save_solution(...)

/* XBraid specific spatial
interpolation/coarsening */
void interpolate_1D(...)
void coarsen_1D(...)
```

ex-02.c

```
typedef struct _braid_App_struct
 MPI_Comm  comm;
 double    matrix[3];
 ...

typedef struct _braid_Vector_struct
 int     size;
 double *values;

int my_Step(u, ...)
 take_step(u->values, ...);

int my_Access(u, ...)
 compute_error_norm(u->values, ...);
 save_solution(fname, u->values, ...);

int my_Init(u, ...)
 get_solution(u->values, ...);

main()
 braid_Core core; app = (my_App *) ...
 braid_Init(..., core);
 braid_Drive(core);
```

Various wrapper functions re-use library routines

How to convert a user-code

- File: `examples/ex-02*`

Solves: $u_t = -u_{xx}$

ex-serial.c

```
  Serial
  Driver
   ...
```

ex-02-lib.c

```
/* Common functions with XBraid */

/* Initialization routine */
void get_solution(...)

/* Helpers for take_step */
void solve_tridiag(...)
void matvec_tridiag(...)
void compute_stencil(...)

/* Core time-stepping routine */
void take_step(...)

/* Output Functions */
double compute_error_norm(...)
void save_solution(...)

/* XBraid specific spatial
interpolation/coarsening */
void interpolate_1D(...)
void coarsen_1D(...)
```

ex-02.c

```
typedef struct _braid_App_struct
 MPI_Comm  comm;
 double    matrix[3];
 ...

typedef struct _braid_Vector_struct
 int     size;
 double *values;

int my_Step(u, ...)
 take_step(u->values, ...);

int my_Access(u, ...)
 compute_error_norm(u->values, ...);
 save_solution(fname, u->values, ...);

int my_Init(u, ...)
 get_solution(u->values, ...);

main()
 braid_Core core; app = (my_App *) ...
 braid_Init(..., core);
 braid_Drive(core);
```

Actually running XBraid is easy!

How to convert a user-code

- File: `examples/ex-02*`

Solves: $u_t = -u_{xx}$

ex-serial.c

```
Serial
Driver
 ...
```

ex-02-lib.c

```
/* Common functions with XBraid */

/* Initialization routine */
void get_solution(...)

/* Helpers for take_step */
void solve_tridiag(...)
void matvec_tridiag(...)
void compute_stencil(...)

/* Core time-stepping routine */
void take_step(...)

/* Output Functions */
double compute_error_norm(...)
void save_solution(...)

/* XBraid specific spatial
interpolation/coarsening */
void interpolate_1D(...)
void coarsen_1D(...)
```

ex-02.c

```
typedef struct _braid_App_struct
 MPI_Comm  comm;
 double    matrix[3];
 ...

typedef struct _braid_Vector_struct
 int     size;
 double *values;

int my_Step(u, ...)
 take_step(u->values, ...);

int my_Access(u, ...)
 compute_error_norm(u->values, ...);
 save_solution(fname, u->values, ...);

int my_Init(u, ...)
 get_solution(u->values, ...);

main()
 braid_Core core; app = (my_App *) ...
 braid_Init(..., core);
 braid_Drive(core);
```

```
$ ex-02 -ntime 64 -nspace 17; python viz-ex-02.py
```

How to debug your new code

- File: `examples/ex-02.c` Solves: $u_t = -u_{xx}$

There is a test function for each wrapper, e.g., `braid_TestInit()`

```
$./ex-02 -wrapper_tests
  ...
  Finished braid_TestAll: no fails detected
```

Set `max-levels=1`. The answer should exactly match sequential time stepping.

```
$ ./ex-02 -ntime 64 -nspace 17 -ml 1
$ python viz-ex-02.py
  (In reality, you'd want to check the agreement to 15 or 16 decimals)
```

Continue with `max-levels=1`, but switch to multiple processors in time. Check that the answer again exactly matches sequential time stepping.

```
$ mpirun -np 2 ex-02 -ntime 64 -nspace 17 -ml 1
$ python viz-ex-02.py
  (In reality, you'd want to check the agreement to 15 or 16 decimals)
```

How to debug your new code

- File: `examples/ex-02.c` Solves: $u_t = -u_{xx}$

Check that XBraid is a fixed point method
Set `max-levels=2`, `tol=0.0`, `max-iter=3`, and initialize XBraid with the sequential solution

```
$ ./ex-02 -ntime 64 -nspace 17 -ml 2 -tol 0.0 -mi 3 -use_seq
  Braid: || r_0 || = 0.000000e+00, conv factor = 1.00e+00, wall time = ...
  Braid: || r_1 || = 0.000000e+00, conv factor = nan, wall time = ...
  Braid: || r_2 || = 0.000000e+00, conv factor = nan, wall time = ...
  Braid: || r_3 || = 0.000000e+00, conv factor = nan, wall time = ...
  Braid: || r_4 || = 0.000000e+00, conv factor = nan, wall time = ...
```

How to debug your new code

- File: `examples/ex-02.c` Solves: $u_t = -u_{xx}$

Turn on debug-level printing and check that the exact solution is propagating

With FCF-relaxation, the exact solution propagates forward 2 C-points each iter

```
$./ex-02 -ntime 8 -nspace 17 -mi 3 -print_level 2
 Braid:  time step:      0, rnorm: 0.00e+00
 Braid:  time step:      2, rnorm: 0.00e+00
 Braid:  time step:      4, rnorm: 6.86e-01
 Braid:  time step:      6, rnorm: 1.10e+00
 Braid:  time step:      8, rnorm: 2.04e-02
 Braid: || r_0 || = 1.292837e+00, conv factor = 1.00e+00, wall time = ...
 Braid:  time step:      0, rnorm: 0.00e+00
 Braid:  time step:      2, rnorm: 0.00e+00
 Braid:  time step:      4, rnorm: 0.00e+00
 Braid:  time step:      6, rnorm: 0.00e+00
 Braid:  time step:      8, rnorm: 1.62e-02
 ...
```

Then, run some larger, multilevel tests of XBraid, checking that the sequential and time-parallel versions agree to within the halting tolerance

Intrusiveness versus efficiency

- The more intrusive XBraid is allowed to be, the more efficient it is
  - **Residual option:** computing the residual with a naive implementation of XBraid is as expensive in FLOPs as sequential time stepping. Writing this extra function allows you to avoid this for implicit schemes.
    - This function also allows relaxation to be significantly less expensive
  - **Adaptivity:** constructing the correct adaptive space-time grid is active research
    - For instance a development branch is currently using threshhold refinement across the temporal communicator to choose time intervals to refine
  - **Storage:** requires a little extra coding, i.e., a new initial guess for implicit scheme
  - **Level-dependent time-stepper:** how to change `Step()` on coarse-levels is problem dependent, but almost always yields big benefits, e.g, vary the tolerance
  - **Spatial coarsening:** this can affect convergence, but is required for an $O(N)$ method in both time and space
  - **Stephanie Friedhoff's talk** covers this in more detail, e.g., results from taking a naive XBraid implementation and moving to an STMG (space-time MG) method

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   → Defining the `App` and `vector` structures, writing wrapper functions, running XBraid
3. Explore more XBraid settings in `examples/ex-01-expanded.c`
4. Porting a user-code to XBraid with `examples/ex-02`
   → Debugging the connection to XBraid
   → Intrusiveness versus efficiency
5. A few application area highlights

Appendix: *Advanced XBraid features*

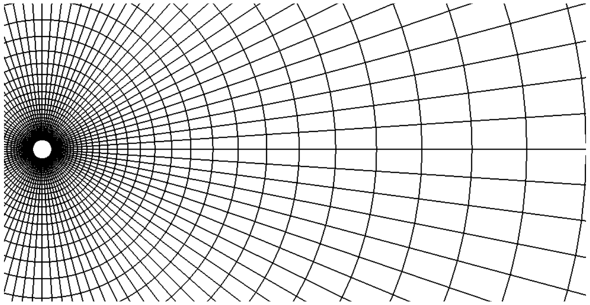
- *Temporal adaptivity*
- *Shell-vectors and BDF-k*
- *Fortran90 Interface*
- *Residual and storage options*
- *Spatial coarsening*

Experiments coupling our code XBraid with various application research codes

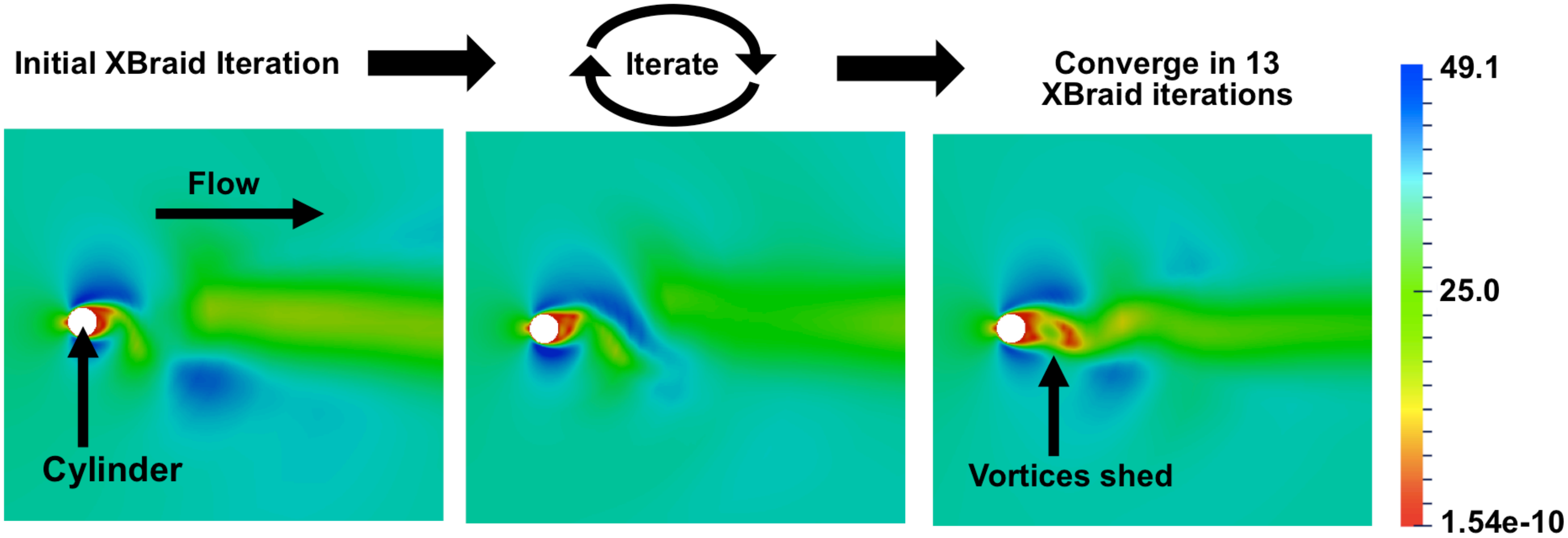
- Navier-Stokes (compressible and incompressible)
  - Strand2D, CarT3D, LifeV (Trilinos-based)
- Heat equation (including moving mesh example)
  - MFEM, hypre
- Nonlinear diffusion, the p-Laplacian
  - MFEM
- Power-grid simulations (project just starting)
  - GridDyn
- Explicit time-stepping coupled with space-time coarsening
  - Heat equation
  - Advection plus artificial dissipation
  - MFEM, hypre

Compressible Navier-Stokes (nonlinear) – speedups to 7.5x with typical MG scaling

- Coupled XBraid with existing code Strand2D (DoD project)
  - ~500 lines of XBraid wrapper code plus minor changes to Strand2D
  - ~3 weeks with minimal outside help

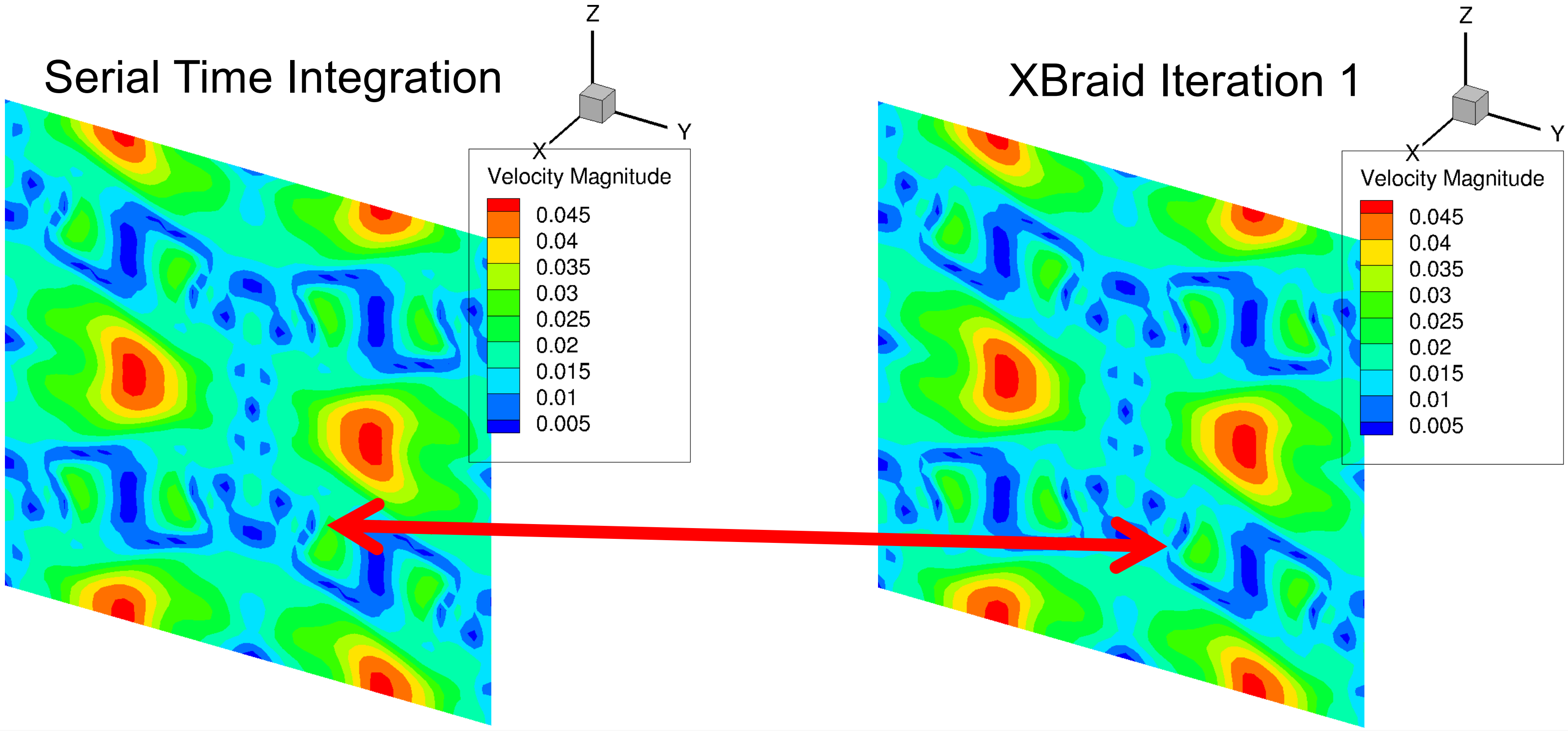


- Plots of velocity magnitude at time step 5120



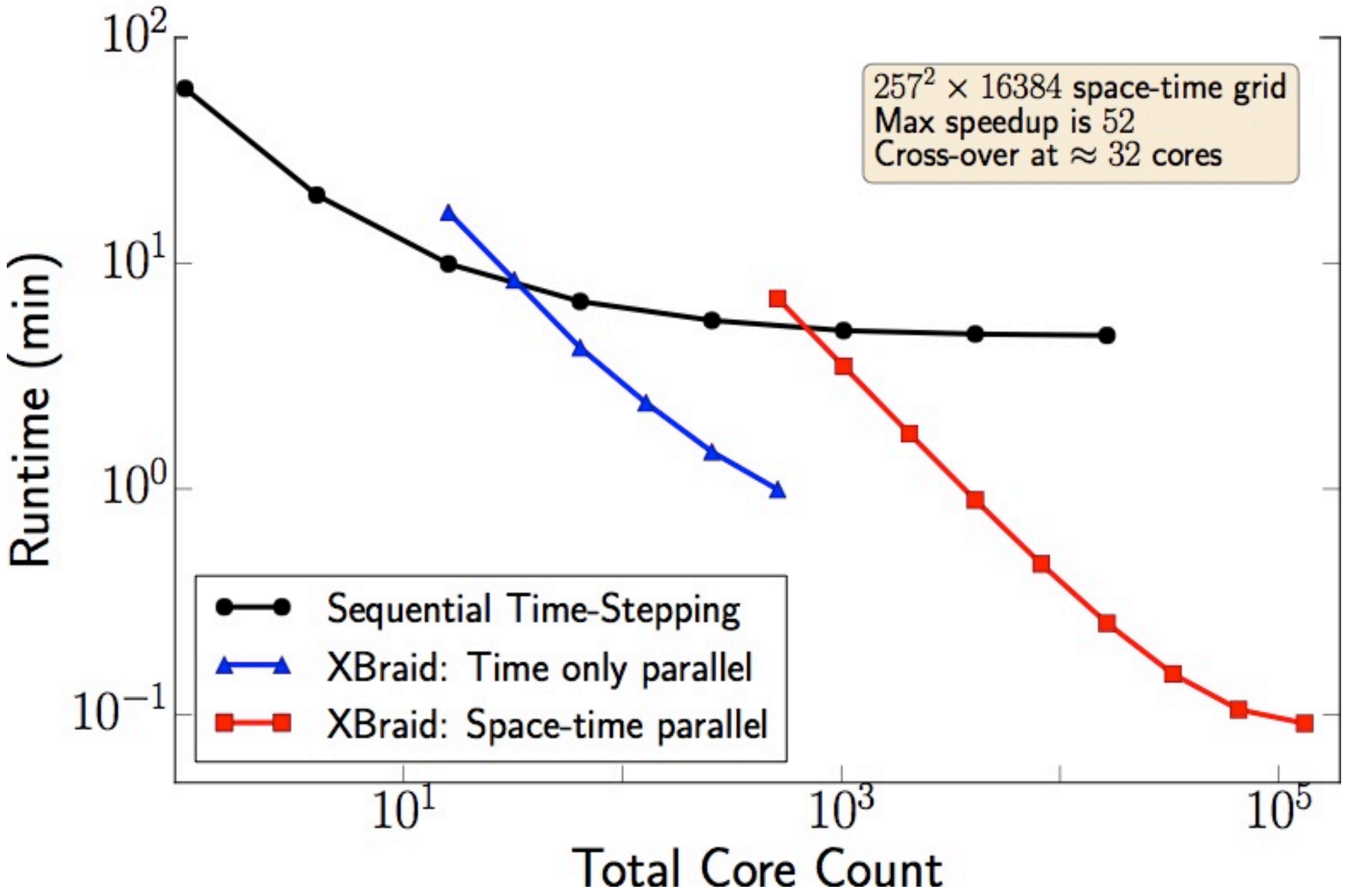
Compressible Navier-Stokes with Cart3D – convergence is very fast, ~5 iterations

- Taylor-Green problem: turbulent decay of vortex, $Re=1600$
  - Higher-order spatial discretization on 58^3 x 20,000 cartesian grid
- Plot velocity magnitude at $x=0$ cross-section



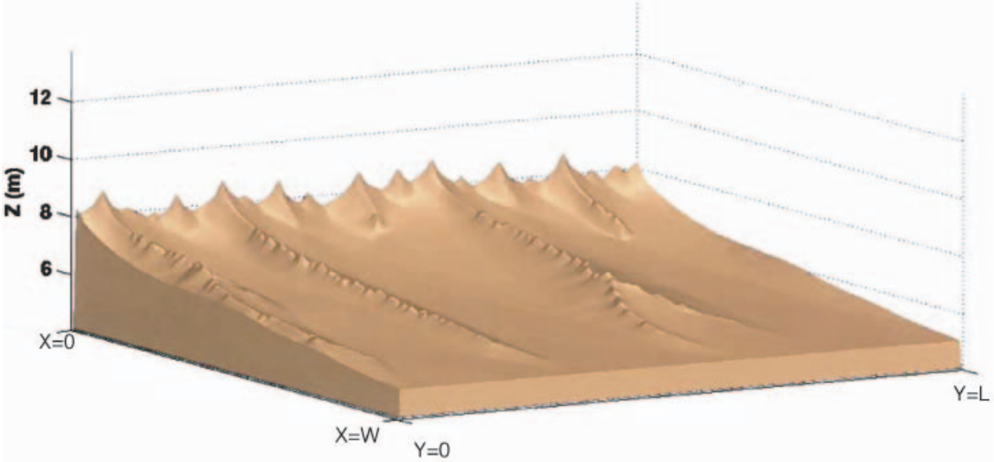
Strong scaling for heat equation

- XBraid uses V-cycles and FCF-relaxation
- Excellent strong scaling, until parallelism is exhausted



The p-Laplacian: nonlinear diffusion

- Solve $u_t = \nabla \cdot \left(|\nabla u|^{p-2}\nabla u\right)$
- 2D linear finite elements
  - 16K x 20K space-time problem
  - Backward Euler (Newton's method)
- Current results
  - Crossover at ~40 processors in time
  - Speedup of 18x at 130K cores
- Important parameters for performance
  - Full storage and space-time coarsening
  - Adjusting the Newton tolerance for the early iterations



Surface Erosion

+++ Image courtesy of Birnir, Rowlett. "Mathematical Models for Erosion and the optimal Transportation of Sediment. Int. J. Nonlinear Sci. Numer. Simul. 2013

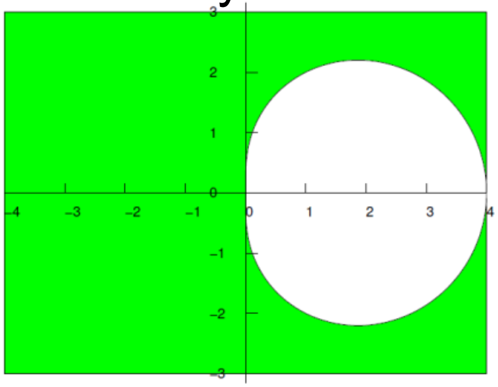
Initial speedups for power-grid

- Simulate 4 generators (30 unknowns) for 30s with 30K time steps

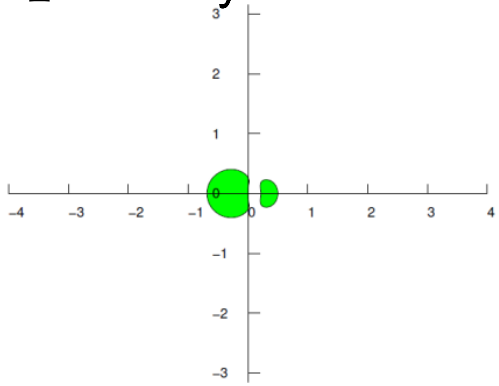
	Sequential	128 cores	256 cores	512 cores	1024 cores
Implicit RK4	**227s**	144s	113s	**102s**	105s
BDF-4	**12.4s**	13.6s	9.46s	7.73s	**7.30s**

- XBraid is designed for one-step methods, so we make BDF-k “one-step” by grouping k time-steps together
  - Creates non-uniform time-step sizes on coarse grids and stability issues for Φ

Φ stability on level 0



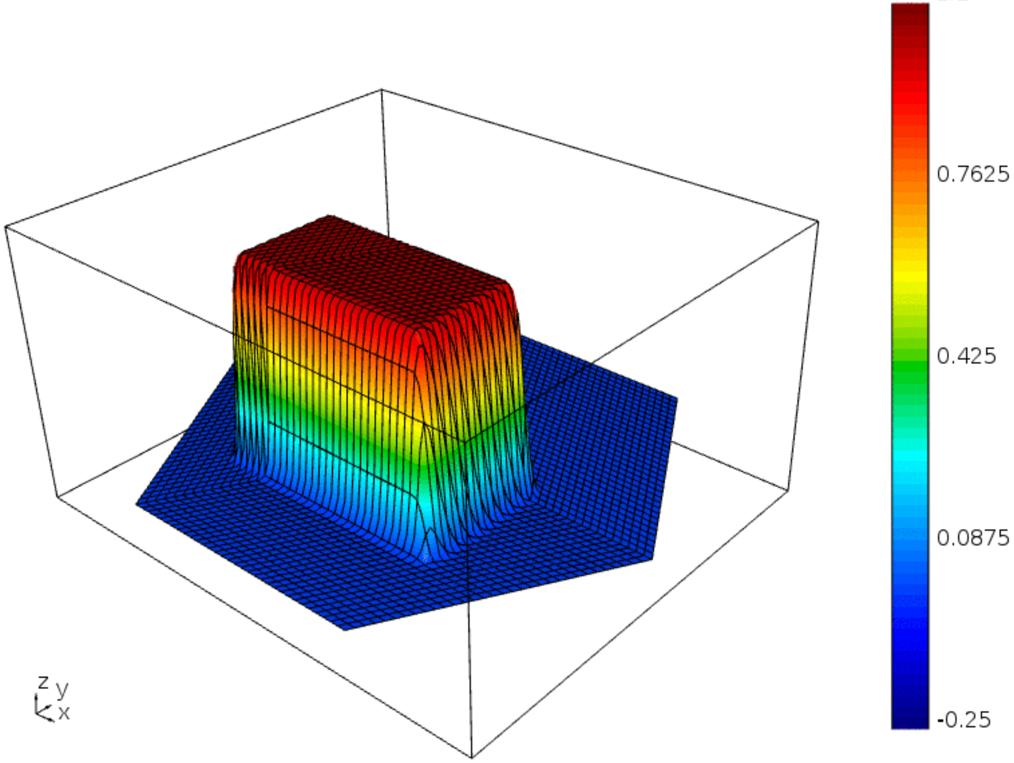
Φ stability on level 3



Solution: reduce the BDF order on coarse levels

Explicit methods with MFEM

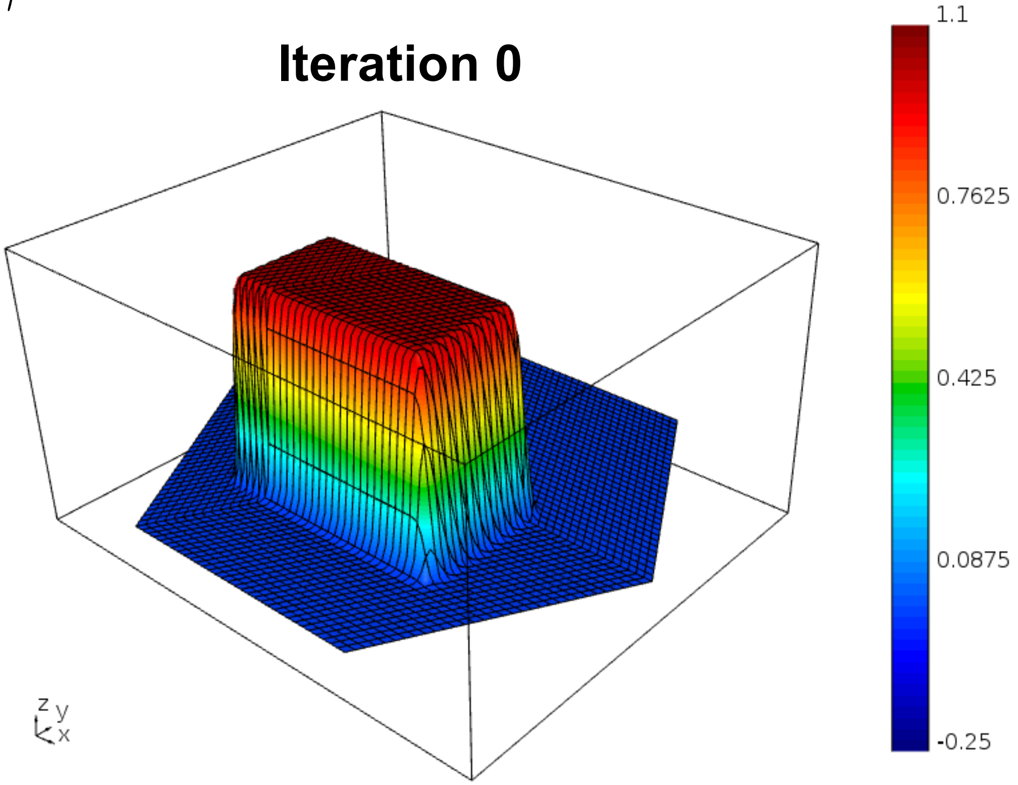
- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
- **Sequential Time Stepping**
  - Sharp profile is transported over 1100 time steps
  - 3rd order explicit method



Explicit methods with MFEM

- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
- **Parallel-in-time solution**
  - Sharp profile is transported over 1100 time steps
  - 3^{rd} order explicit method
  - 3-level XBraid hierarchy

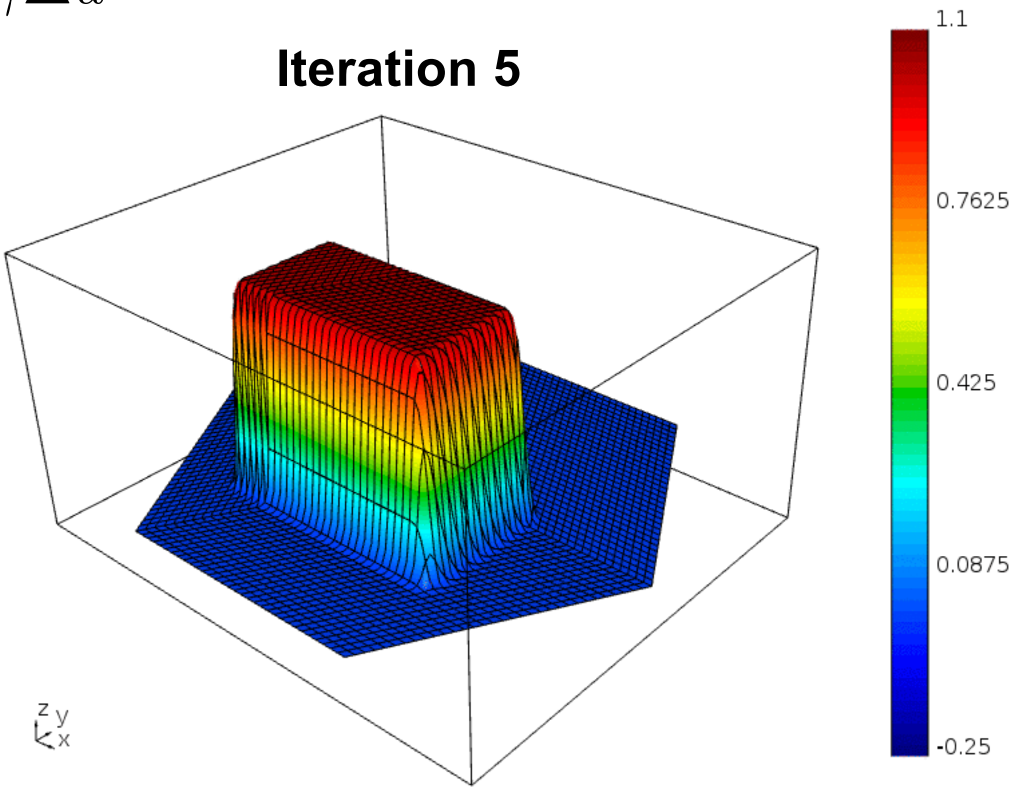
Iteration 0



Explicit methods with MFEM

- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
- **Parallel-in-time solution**
  - Sharp profile is transported over 1100 time steps
  - 3^{rd} order explicit method
  - 3-level XBraid hierarchy

Iteration 5



Explicit methods with MFEM

- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
- **Parallel-in-time solution**
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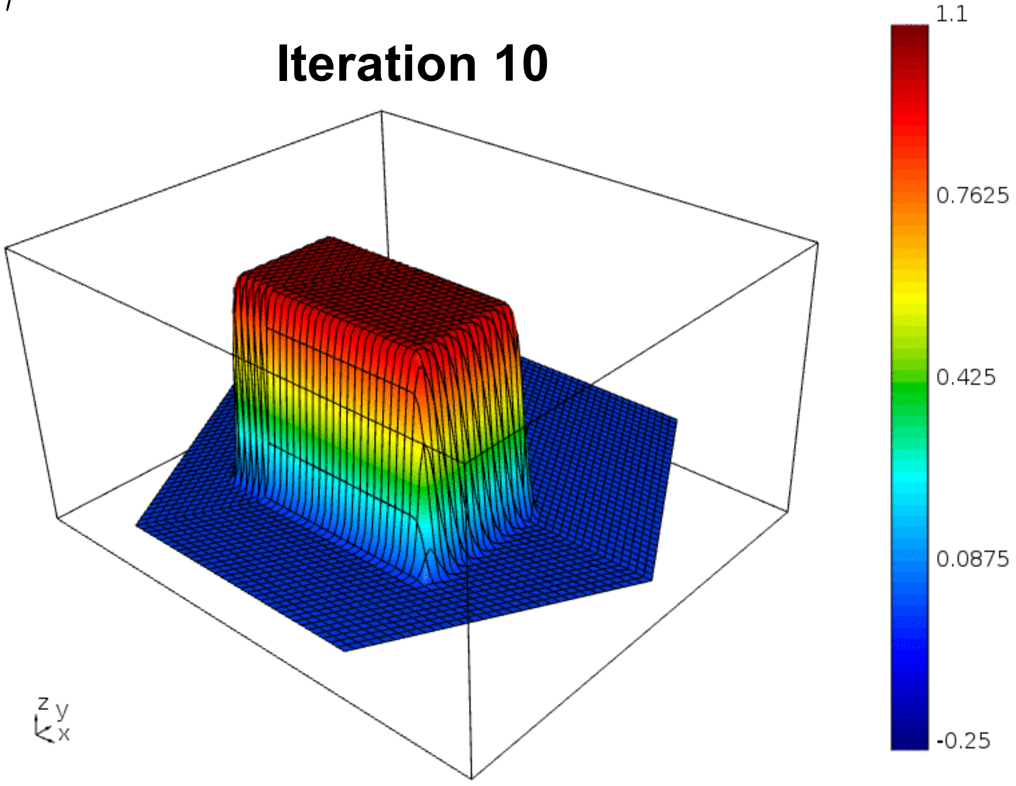
  - 3rd order explicit method
  - 3-level XBraid hierarchy

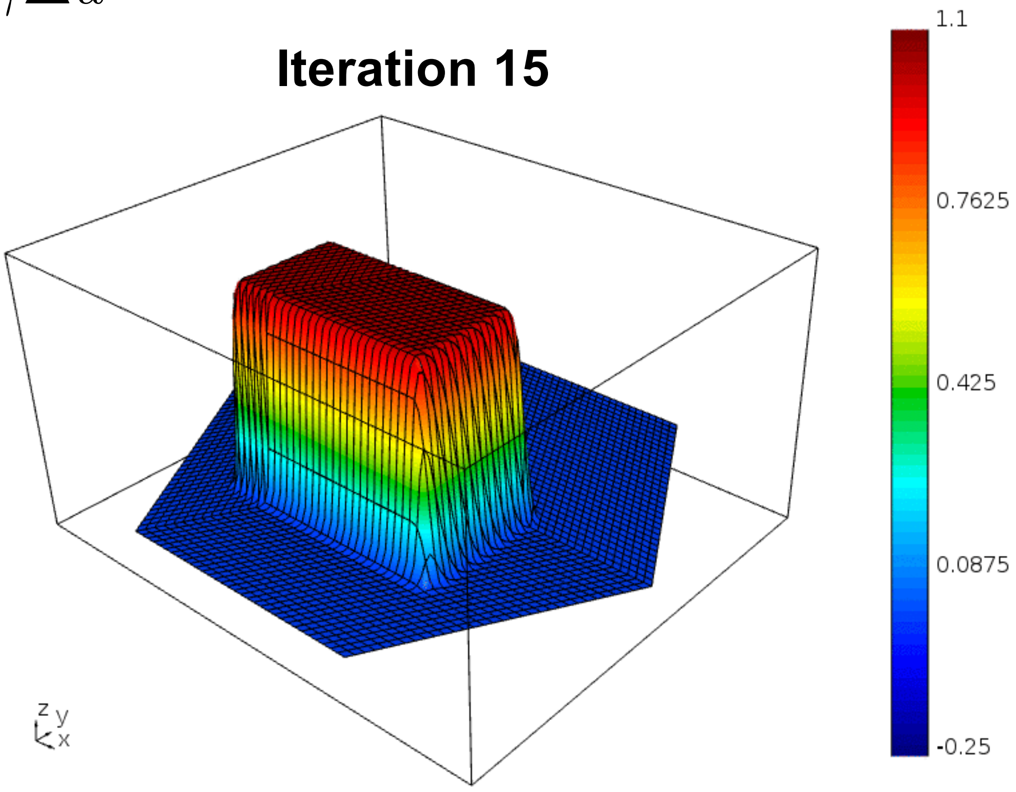
Iteration 10



Explicit methods with MFEM

- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
- **Parallel-in-time solution**
  - Sharp profile is transported over 1100 time steps
  - 3rd order explicit method
  - 3-level XBraid hierarchy

Iteration 15



Explicit methods with MFEM

- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
- **Parallel-in-time solution**
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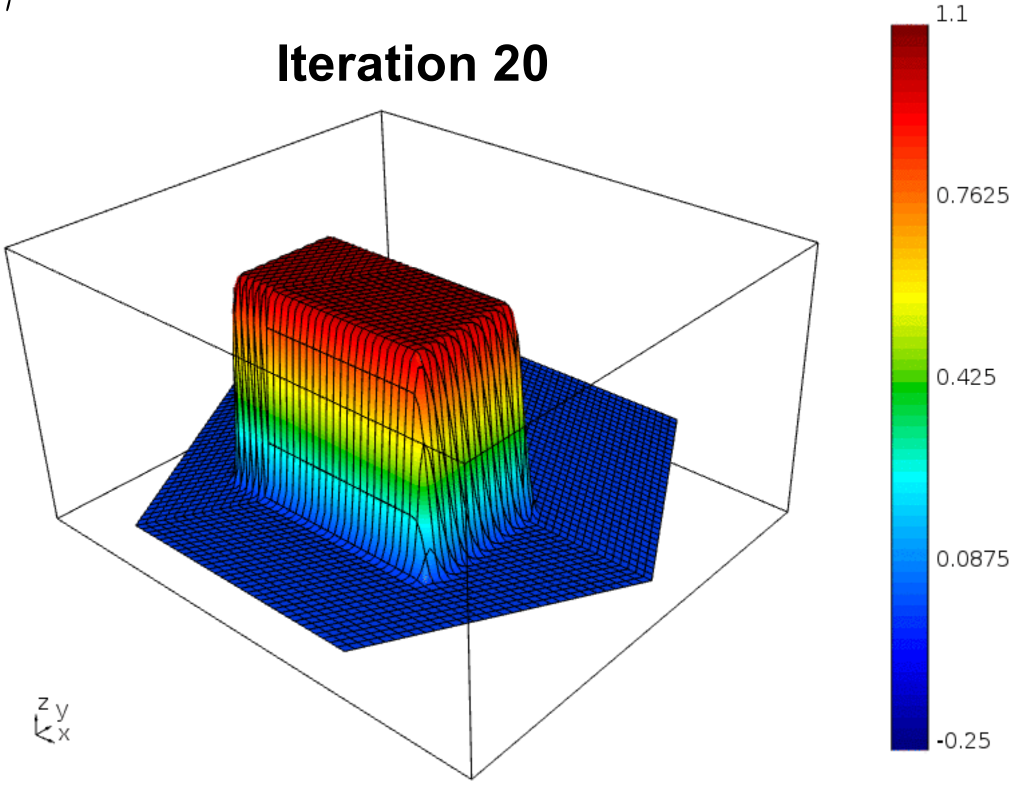
  - 3^{rd} order explicit method
  - 3-level XBraid hierarchy

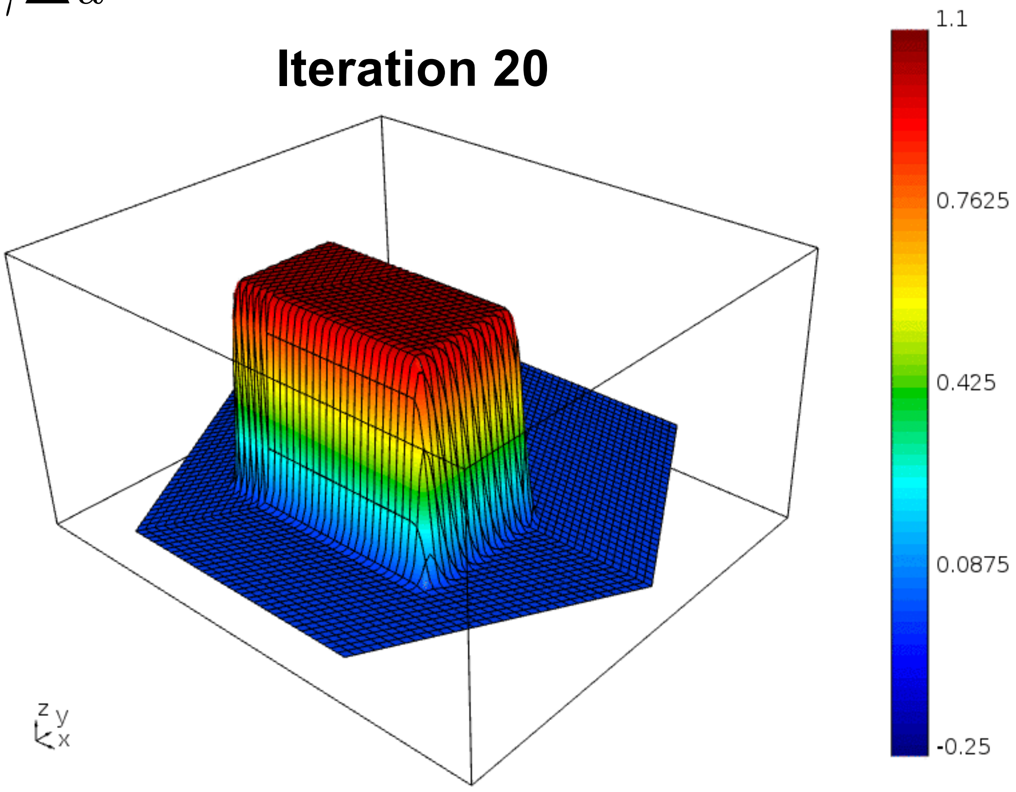
Iteration 20



Explicit methods with MFEM

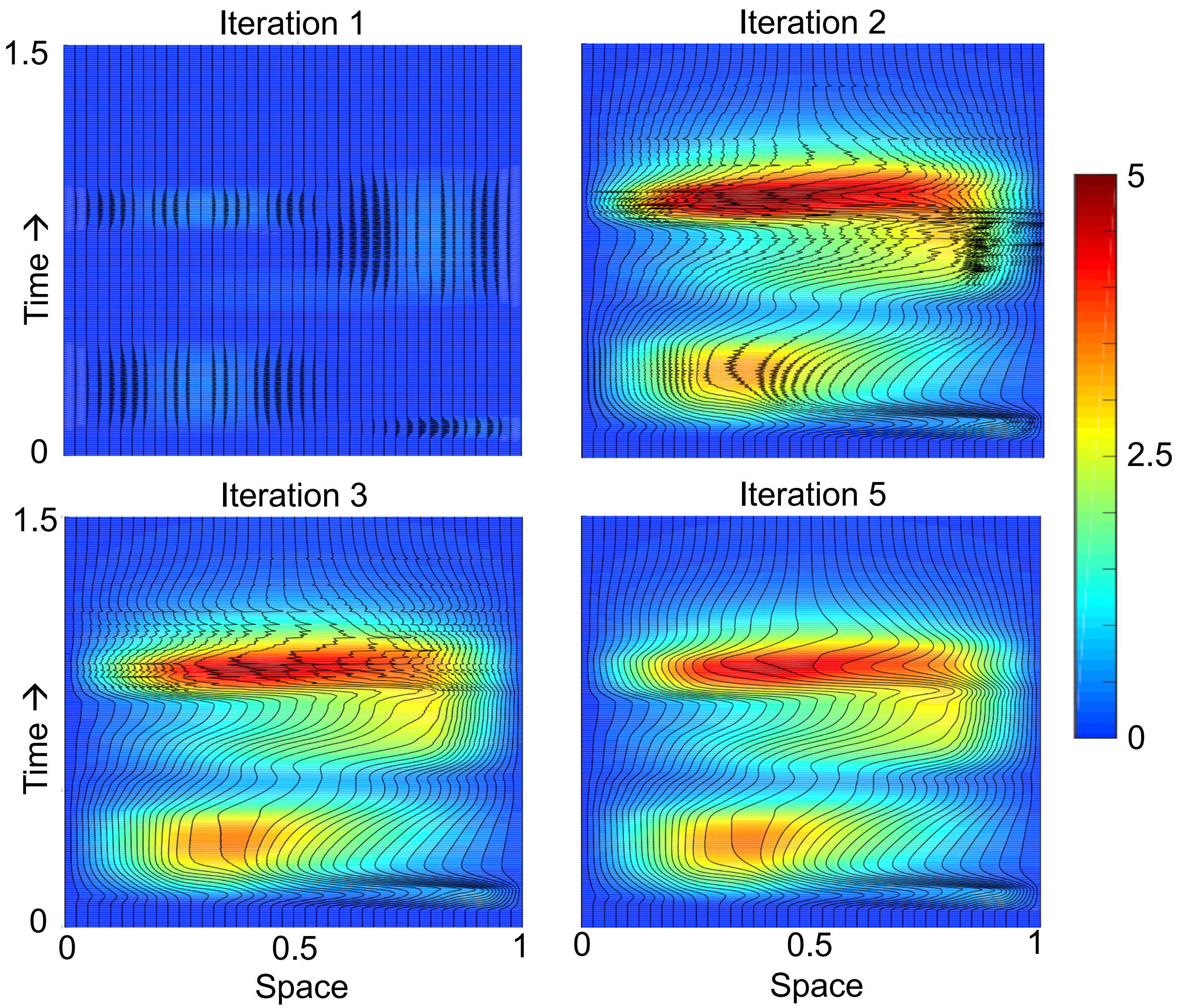
- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
- **Parallel-in-time solution**
  - Sharp profile is transported over 1100 time steps
  - 3rd order explicit method
  - 3-level XBraid hierarchy
- Future Work: Improve convergence (relaxation, coarse-grid equations)

Iteration 20



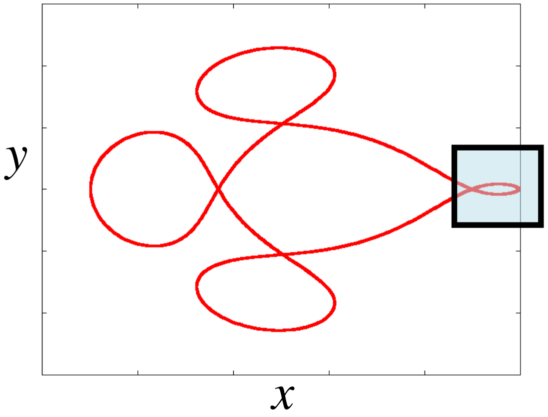
Moving mesh

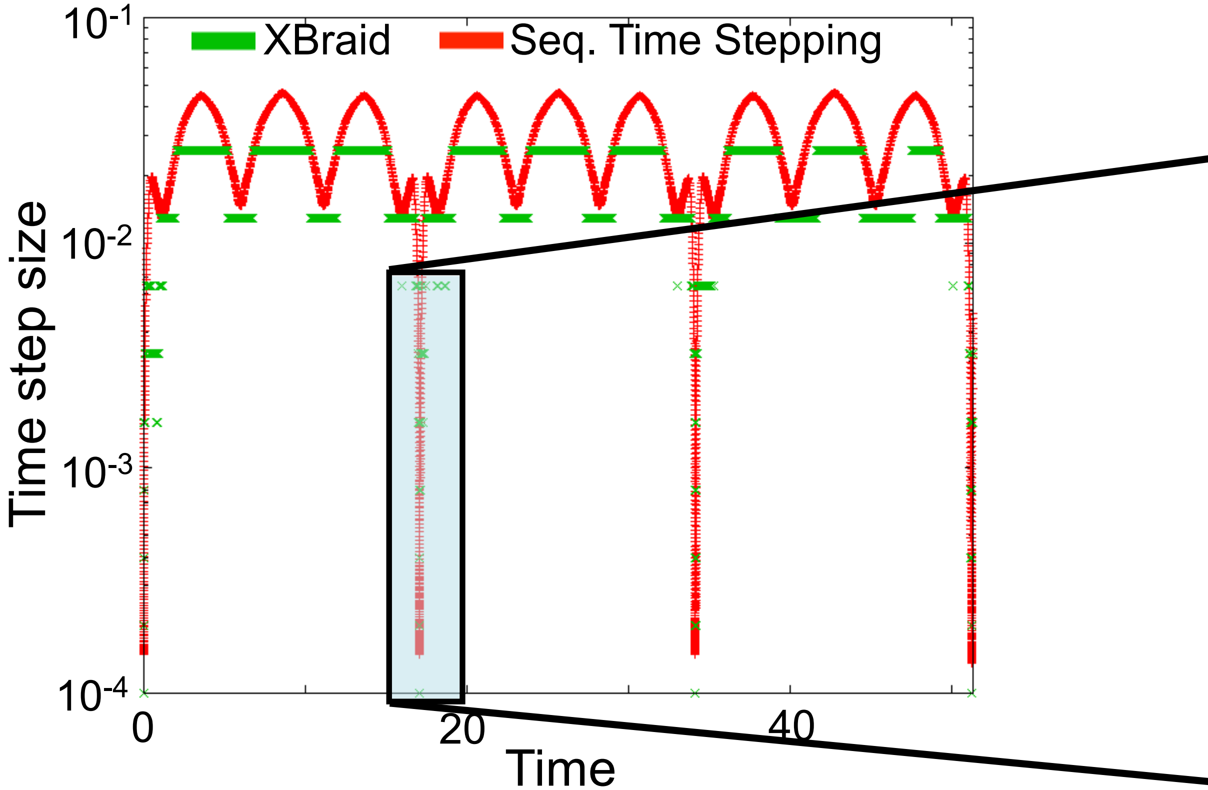
- 1D space moving mesh proof-of-concept
- Mesh points move towards regions with a rapidly changing solution
- Fast convergence and scalable iteration counts
- More complicated moving mesh problems coming...

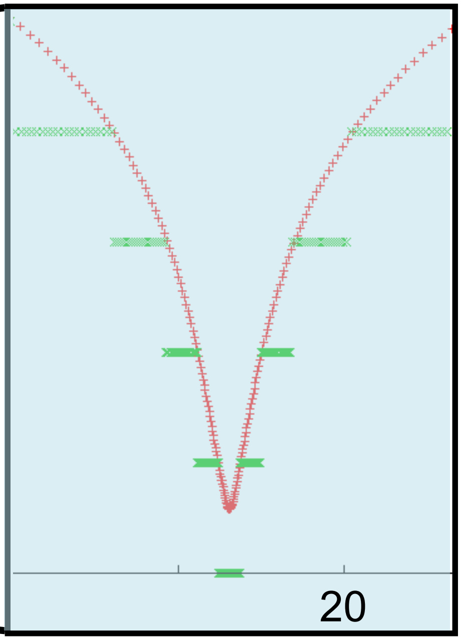


Temporal adaptivity proof-of-concept

- Classic ODE modeling satellite orbit around earth and moon (2 variables in space, x and y)
- One region of orbit requires very fine time steps
  - Carry out 4 periods of orbit, refining step size as needed







Nearly 50 years of research exists, but has only scratched the surface

- Earliest work goes back to 1964 by Nievergelt
  - Led to multiple shooting methods, Keller (1968)
- Space-time multigrid methods for parabolic problems
  - Hackbusch (1984); Horton (1992); Horton and Vandewalle (1995)
  - The latter is one of the first optimal & fully parallelizable methods to date
- Parareal was introduced by Lions, Maday, and Turincini in 2001
  - Probably the most widely studied method
  - Gander and Vandewalle (2007) show that parareal is two-level FAS multigrid
- Discretization specific work includes
  - Minion, Williams (2008, 2010) – PFASST, spectral deferred correction / parareal
  - DeSterck, Manteuffel, McCormick, Olson (2004, 2006) – FOSLS
- Research on these methods is ramping up!
  - Ruprecht, Krause, Speck, Emmett, Langer, … this is not an exhaustive list

Summary and conclusions

- Sequential time integration bottleneck is real
  - Parallel in time is needed for future architectures
  - This is a major paradigm shift

- XBraid applies multigrid reduction to the time dimension
  - Multigrid is ideal for exascale (optimal, resilient, ...)
  - Result is a flexible and non-intrusive approach

- The more intrusive XBraid is allowed to be, the more efficient the algorithm is.

- There is much future work to be done!
  - More problem types, more complicated discretizations, performance improvements, adaptive meshing, ...

Thank You! Any Questions?

A good read, *Parallel Time Integration with Multigrid*, SIAM J. Sci. Comp.

Open Source XBraid Code

- http://llnl.gov/casc/xbraid
- Supports C, C++, F90

XBRAID
PARALLEL MULTIGRID IN TIME

Our Team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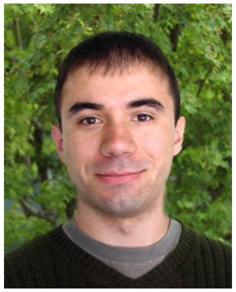
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Collaborators and summer interns

CU Boulder (Manteuffel, McCormick, O'Neill, Southworth), Memorial University (MacLachlan), U Cologne (Friedhoff), U Stuttgart (Hessenthaler), Monash U (De Sterck)

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   → Tutorial software requirements and XBraid overview
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   → Defining the `App` and `vector` structures, writing wrapper functions, running XBraid
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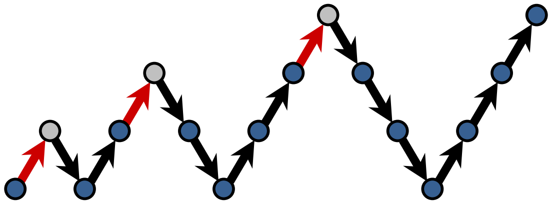
Appendix: *Advanced XBraid features*

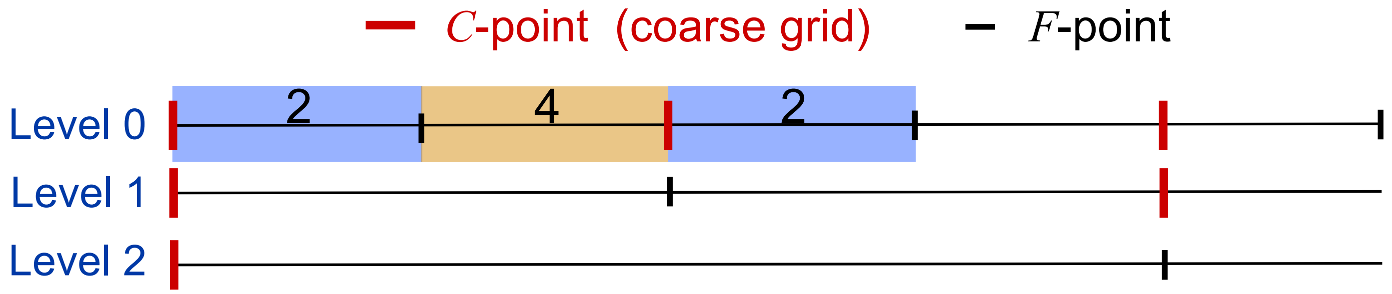
- *Temporal adaptivity*
- *Shell-vectors and BDF-k*
- *Fortran90 Interface*
- *Residual and storage options*
- *Spatial coarsening*

Advanced feature: FMG allows for adaptivity in time and space

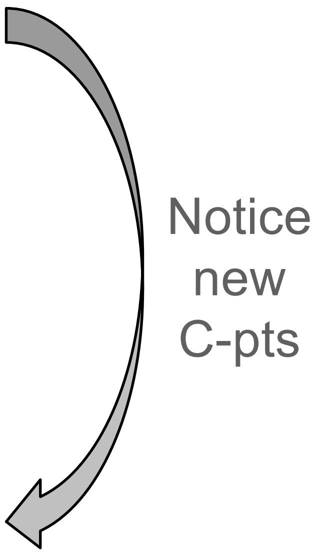
- User returns refinement factor in `Step()`

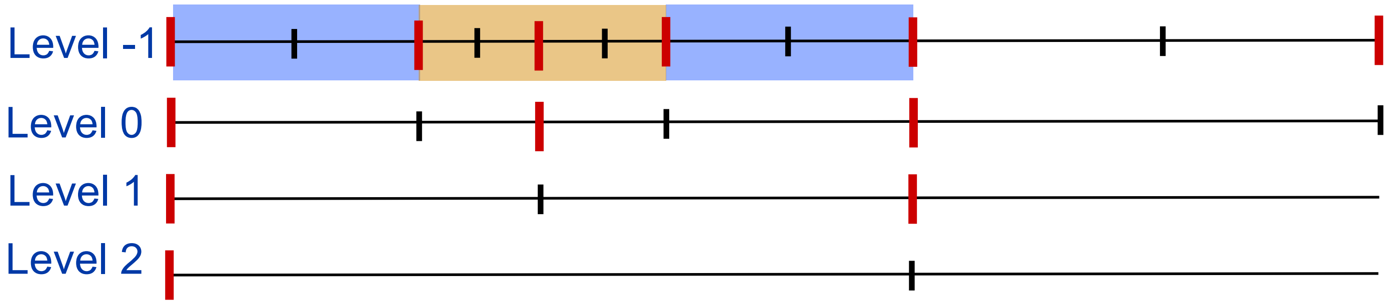


- Example time grid hierarchy



- User requests refinement factors on the finest grid which generates a new grid and hierarchy





Advanced feature: adaptivity in time

- File: `examples/ex-03.c` Solves: $u_t = -u_{xx} - u_{yy}$

- **This simple example carrries out naive pre-specified refinements**
- **`braid_StepStatusSetRFactor(status, k)` refines an interval `k` times**
  - **Called from inside of `Step()`**

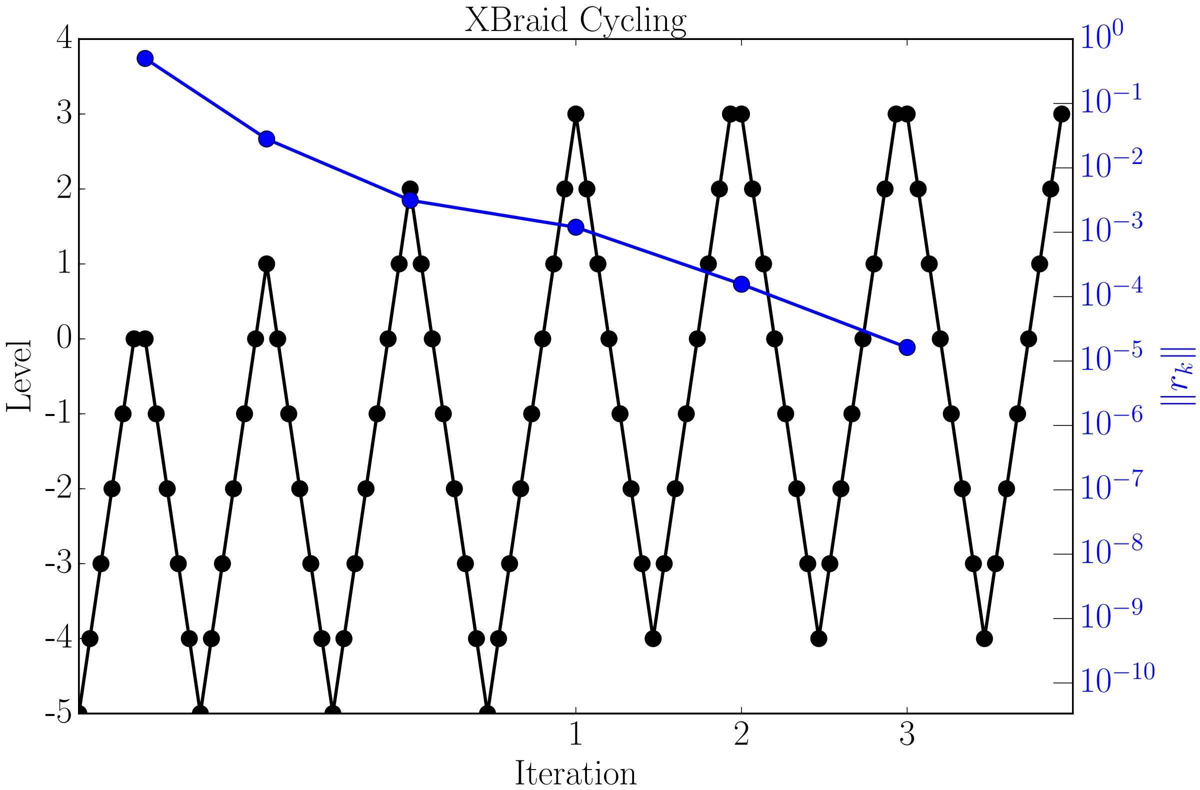
```
$ make ex-03
$ ./ex-03 -nt 128 -nx 9 9 -mi 4 -refine
 Braid: Begin simulation, 128 time steps
 Braid: || r_0 || not available, wall time = ...
 Braid: || r_1 || = 5.002967e-01, conv factor = 1.00e+00, wall time = ...
 Braid: Temporal refinement occurred, 242 time steps

 Braid: || r_1 || = 2.810253e-02, conv factor = 1.00e+00, wall time = ...
 Braid: Temporal refinement occurred, 390 time steps

 Braid: || r_1 || = 3.136143e-03, conv factor = 1.00e+00, wall time = ...
 Braid: Temporal refinement occurred, 583 time steps

 Braid: || r_1 || = 1.197026e-03, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 1.558192e-04, conv factor = 1.30e-01, wall time = ...
 Braid: || r_3 || = 1.623626e-05, conv factor = 1.04e-01, wall time = ...
```

Advanced feature: adaptivity in time

- File: `examples/ex-03.c` Solves: $u_t = -u_{xx} - u_{yy}$

- **Now, visualize the cycling**
- **Observe how the new levels (and time-points) are added**
- **This causes an uneven reduction in the residual**

```
$ python ../user_utils/cycleplot.py
```



Refinement here is with a V-cycle. But can also be done with FMG cycles.

Advanced feature: residual function

- File: `examples/ex-01-expanded.c` Solves: $u_t = \lambda u$

Observe how turning on the residual function changes convergence

```
$./ex-01-expanded -ntime 128 -res
...
iterations                = 7

$./ex-01-expanded -ntime 128
...
iterations                = 6
```

- File: `examples/ex-03.c` Solves: $u_t = -u_{xx} - u_{yy}$

```
$ make ex-03
$ ./ex-03 –res -nt 128 -nx 9 9 -mi 4
 Braid: || r_1 || = 5.231464e-01, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 6.067546e-02, conv factor = 1.16e-01, wall time = ...

$ ./ex-03 -nt 128 -nx 9 9 -mi 4
 Braid: || r_1 || = 5.002967e-01, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 2.701758e-02, conv factor = 5.40e-02, wall time = ...
```

Understanding the residual feature

- XBraid computes the FAS residual in a block-row fashion for the space-time system

$$A_i(\mathbf{u}_i, \mathbf{u}_{i-1}) = f_i$$

- Consider, for example, the common additive form of a user residual:

  User specifies this → $A_i(\mathbf{u}_i, \mathbf{u}_{i-1}) = -\Phi(\mathbf{u}_{i-1}) + \Psi(\mathbf{u}_i)$

  FAS residual computed internally → $r_i = f_i + \Phi(\mathbf{u}_{i-1}) - \Psi(\mathbf{u}_i)$

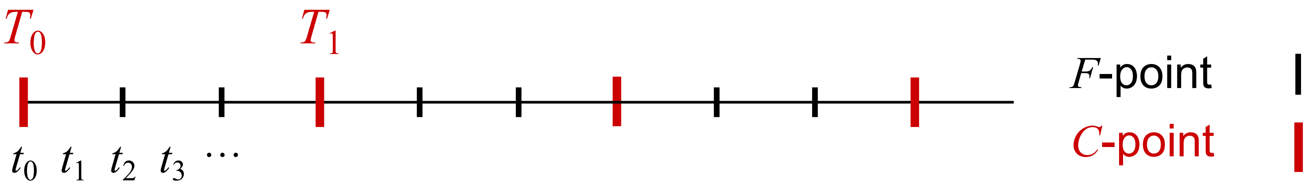
- **Default setting**: `Step()` = $\Phi(\mathbf{u}_i)$ and $\Psi = I$
  - XBraid can compute the rest of the residual on its own

- **Residual setting:** user defines a new function $\texttt{Residual}(\texttt{u}_{\texttt{i}},\ \texttt{u}_{\texttt{i-1}})\ = A_i(\mathbf{u}_i, \mathbf{u}_{i-1})$
  - This function defines the equation to be solved, implying that `Step()` must be compatible.
  - `Step()` must now compute $u_i = \Psi^{-1}(f_i + \Phi(u_{i-1}))$
  - Notice how `Step()` must now account for f_i , that is, `fstop` in `Step()` is no longer NULL!

- **Computational savings:** consider the heat equation and backward Euler
  - **Default:** `Step()` implements Φ, a full implicit solve for an accurate residual
  - **Residual:** `Step()` implements a very weak inexact solve (only used for relaxation)
    `Residual()` uses $\Phi = I$ and Ψ is just a sparse matrix (very cheap!)

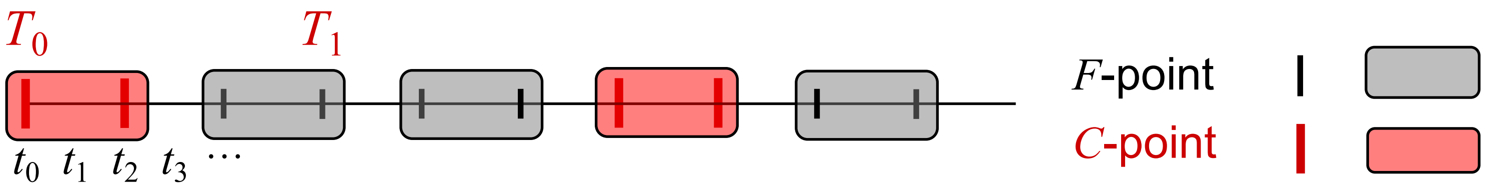
Advanced feature: shell-vectors & BDF-k

- File: `examples/ex-01-expanded-bdf2.c` Solves: $u_t = \lambda u$
- XBraid is designed for one-step methods. This is the standard way to partition the time-line.



Advanced feature: shell-vectors & BDF-k

- File: `examples/ex-01-expanded-bdf2.c` Solves: $u_t = \lambda u$
- XBraid is designed for one-step methods. The new way to partition so that BDF-k looks “one-step” is to group k time-steps together (here, $k = 2$).



  - Creates non-uniform time-step sizes on coarse grids
- The shell-vector feature allows for the storage of meta-data at every time point, including F-points that are otherwise not stored.
  - This meta-data allows for tracking the irregular time-grid spacing
- Other BDF-k strategies, like reducing order on coarse-grids, are possible
- To use the shell option, you must define new shell functions for allocating, copying, and freeing vector shells

Advanced feature: extra storage

- File: `examples/ex-03.c` Solves: $u_t = -u_{xx} - u_{yy}$

- **Set a storage value k (default is *-1*)**
  - ***For level ≥ k ≥ 0, store all points; for level < k, store only C-points***
  - ***k = 0 storage at all points on all levels***
  - ***k = -1 special value, storage only at C-points on all levels***

– F-point (fine grid only)

– C-point (coarse & fine grid)

- **The extra storage critically gives improved initial guesses to implicit solvers**
- **The extra storage changes the problem being solved**
  - **The operator Φ changes as the initial guess changes**

- **Look at the residual histories with**

```
$ make ex-03
$ ./ex-03 -nx 17 17 -nt 128 -storage -1

$ ./ex-03 -nx 17 17 -nt 128 -storage  0

$ ./ex-03 -nx 17 17 -nt 128 -storage  1
```

$$\begin{pmatrix} I & & & \\ -\Phi & I & & \\ & \ddots & \ddots & \\ & & -\Phi & I \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \boldsymbol{u}_1 \\ \vdots \\ \boldsymbol{u}_N \end{pmatrix} = \begin{pmatrix} \boldsymbol{g}_0 \\ \boldsymbol{g}_1 \\ \vdots \\ \boldsymbol{g}_N \end{pmatrix}$$

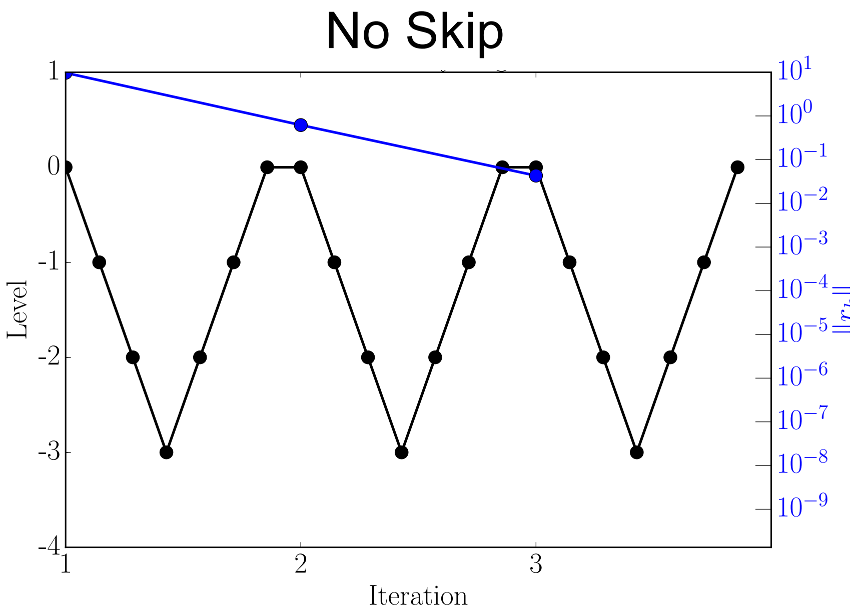
Advanced feature: skip option

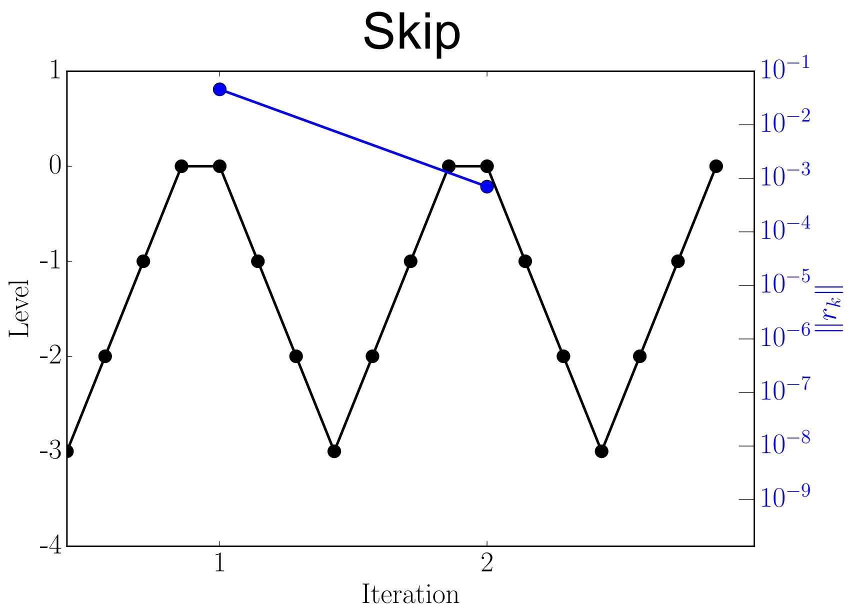
- File: `examples/ex-03.c`

Solves: $u_t = -u_{xx} - u_{yy}$

- **Skip allows XBraid to skip (typically useless) relaxations on the 1st down cycle**
    - **By default, skip is turned on**
- **Compare the residual histories for**

```
$ ./ex-03 -nx 17 17 -nt 128 -skip 1
$ ./ex-03 -nx 17 17 -nt 128 -skip 0
```


No Skip


Skip

Advanced feature: parallel-run

- File: `examples/ex-03.c` Solves: $u_t = -u_{xx} - u_{yy}$

Run in parallel!

```
$./mpirun -np 8 ex-03 -pgrid 2 2 2 -nt 256 -nx 17 17
 Braid: || r_0 || not available, wall time = ...
 Braid: || r_1 || = 6.166798e-01, conv factor = 1.00e+00, wall time = ...
 Braid: || r_2 || = 2.319985e-02, conv factor = 3.76e-02, wall time = ...
 Braid: || r_3 || = 6.972052e-04, conv factor = 3.01e-02, wall time = ...
 Braid: || r_4 || = 1.135286e-05, conv factor = 1.63e-02, wall time = ...
 ...
```

Advanced feature: spatial coarsening

- File: `examples/ex-02.c`

Solves: $u_t = -u_{xx}$

Here, we use simple bilinear interpolation (and its transpose) for spatial coarsening

```
$./ex-02 -ntime 64 -nspace 17 -ml 3 -sc
 Braid: || r_0 || = 2.935397e+00, conv factor = 1.00e+00, wall time = ...
 Braid: || r_1 || = 1.483600e-01, conv factor = 5.05e-02, wall time = ...
 Braid: || r_2 || = 3.884625e-03, conv factor = 2.62e-02, wall time = ...
 Braid: || r_3 || = 1.315185e-04, conv factor = 3.39e-02, wall time = ...
 ...
  level       dx           dt         dt/dx^2
 -----------------------------------------------------------------
   0    |   1.96e-01    9.82e-02    2.55e+00
   1    |   3.93e-01    1.96e-01    1.27e+00
   2    |   7.85e-01    3.93e-01    6.37e-01
```

Spatial coarsening is active research and can (sometimes) negatively impace convergence.

```
$./ex-02 -ntime 64 -nspace 17 -ml 3
 Braid: || r_0 || = 2.935397e+00, conv factor = 1.00e+00, wall time = ...
 Braid: || r_1 || = 1.666814e-01, conv factor = 5.68e-02, wall time = ...
 Braid: || r_2 || = 8.328760e-03, conv factor = 5.00e-02, wall time = ...
 Braid: || r_3 || = 2.844685e-04, conv factor = 3.42e-02, wall time = ...
 ...
  level      dx           dt          dt/dx^2
 -----------------------------------------------------------------
   0    |   1.96e-01    9.82e-02    2.55e+00
   1    |   1.96e-01    1.96e-01    5.09e+00
   2    |   1.96e-01    3.93e-01    1.02e+01
```

Advanced feature: coarsening factor

- File: `examples/ex-02.c` Solves: $u_t = -u_{xx}$

- **Changing the coarsening factor does not change convergence (much)**
- **This powerful fact applies to parabolic problems in general**
  - **Allows for a great deal of performance tuning**
  - **Requires that FCF-relaxation or F-cycles be used**

```
$./ex-02 -ntime 1024 -nspace 128 -cf 16 -ml 10
...
iterations                 = 7

$./ex-02 -ntime 1024 -nspace 128 -cf 2 -ml 10
...
iterations                 = 8
```

Fortran90 interface

- File: `examples/ex-01-expanded-f.f90` Solves: $u_t = \lambda u$

Uses Fortran90 modules to define the App and Vector Types

```
module braid_types

   type my_vector
      double precision val
   end type my_vector
   ...
```

User-defined wrapper functions are the same, only written in Fortran90

```
subroutine braid_Sum_F90(app, alpha, x, beta, y)
   ! Braid types
   use braid_types
   implicit none
   type(my_vector)          :: x, y
   type(my_app)             :: app

   double precision alpha, beta
   y%val = alpha*(x%val) + beta*(y%val)
end subroutine braid_Sum_F90
```