Parallel in Time with SUNDIALS and XBraid

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SUNDIALS: SUite of Nonlinear and Differential / ALgebraic equation Solvers

- Software library of ODE and DAE time integrators and nonlinear solvers
  - Consists of six packages: CVODE(S), **ARKode**, IDA(S), and KINSOL
  - Written in C with interfaces to Fortran
  - *Designed to be easily incorporated into existing codes*
- Modular implementation
  - Data use is fully encapsulated by vector and matrix APIs
  - Nonlinear and linear solvers are fully encapsulated from the integrators
  - All parallelism is encapsulated in vectors, solvers, and user-supplied functions
  - *Vector, matrix, and solver modules can all be user-supplied*
- Availability and support
  - Freely available; BSD 3-Clause license; >27,000 downloads in 2019
  - Detailed user manuals and an active user community email list

https://computing.llnl.gov/sundials

ARKode – Adaptive Runge-Kutta methods

- The ARKode package is designed to work as an infrastructure for developing adaptive one-step time integration methods.
  - **ARKStep:** Provides ERK, DIRK, and IMEX ARK methods for problems of the form

$$M\frac{dy}{dt} = f^E(t,y) + f^I(t,y), \qquad y(t_0) = y_0$$

  - **ERKStep**: A streamlined module for ERK methods for problems of the form

$$\frac{dy}{dt} = f(t,y), \qquad y(t_0) = y_0$$

  - **MRIStep:** Multirate Infinitesimal Step (MIS) like methods for problems of the form

$$\frac{dy}{dt} = f^F(t,y) + f^S(t,y), \qquad y(t_0) = y_0$$

ARKStep – Additive Runge-Kutta methods

- IMEX ARK methods for problems with two split components:

$$M\frac{dy}{dt} = f^E(t,y) + f^I(t,y), \qquad y(t_0) = y_0$$

  - M is any nonsingular linear operator (mass matrix, typically $M = I$),
  - $f^E(t,y)$ contains the explicit (non-stiff) terms,
  - $f^I(t,y)$ contains the implicit (stiff) terms.

- Combine two s-stage RK methods; let $t^*_{n,j} = t_n + c_j h_n$, $h_n = t_{n+1} - t_n$:

$$Mz_i = My_n + h_n \sum_{j=1}^{i-1} A^E_{i,j} f^E\left(t^E_{n,j}, z_j\right) + h_n \sum_{j=1}^{i} A^I_{i,j} f^I\left(t^I_{n,j}, z_j\right), \qquad i = 1, \ldots, s$$

$$My_{n+1} = My_n + h_n \sum_{j=1}^{s} b^E_j f^E\left(t^E_{n,j}, z_j\right) + b^I_j f^I\left(t_{n,j}, z_j\right) \qquad \text{(solution)}$$

$$M\tilde{y}_{n+1} = My_n + h_n \sum_{j=1}^{s} \tilde{b}^E_j f^E\left(t^E_{n,j}, z_j\right) + \tilde{b}^I_j f^I\left(t_{n,j}, z_j\right) \qquad \text{(embedding)}$$

Time steps are chosen to minimize local truncation error and maximize efficiency

- All SUNDIALS integrators utilize local truncation error estimates to adapt the step size to meet user defined tolerances

$$w_i = \frac{1}{rtol\ |y_i| + atol_i} \qquad \|y\|_{wrms} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(w_i y_i)^2}$$

  - With Runge-Kutta methods the error estimate is based on the difference between the computed and embedded solutions
  - Accept the step if $\|E(h_n)\|_{wrms} < 1$, otherwise reject the step
  - Choose h_{n+1} such that $\|E(h_{n+1})\| < 1$

- Relative tolerance ($rtol$) controls local error relative to the size of the solution
  - $rtol = 10^{-4}$ means that errors are controlled to 0.01%

- Absolute tolerances ($atol$) control error when a solution component may be small
  - e.g., $atol_i$ should be the noise level for a solution component

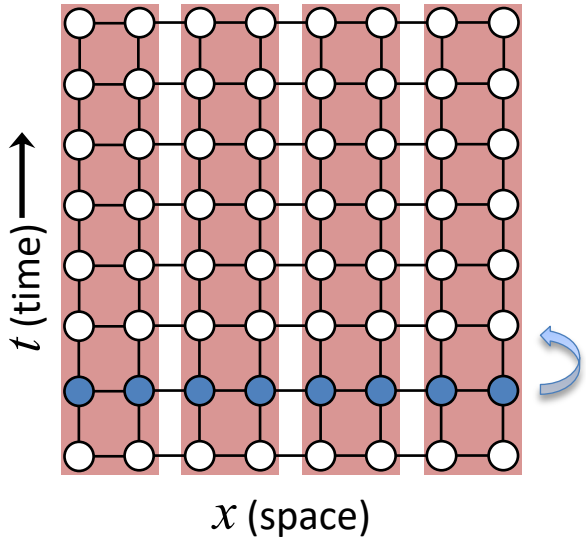
ARKode Flexibility Features

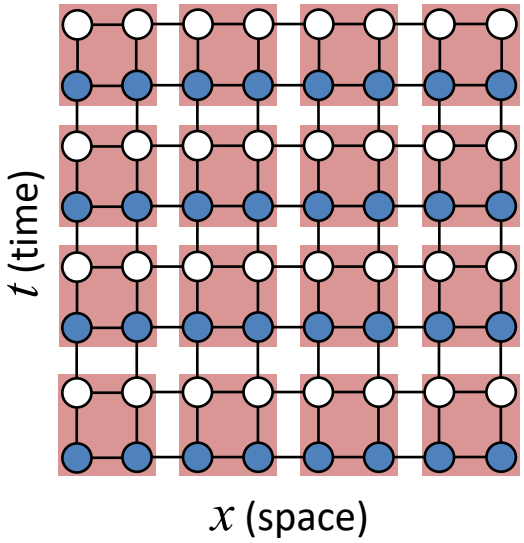
- Built on SUNDIALS vector, matrix, and solver APIs:
  - Several native modules including wrappers to other math libraries
  - Supports user defined modules

- ARKode includes several additional enhancements including:
  - Variety of built-in Butcher tables (ERK, DIRK, & IMEX) or user-supplied
  - Variety of built-in step size adaptivity controllers, or user-supplied
  - Variety of built-in implicit predictor algorithms, or user-supplied
  - Ability to specify that problem is linearly implicit
  - Ability to resize data structures based on changing IVP size
  - All internal solver parameters are user-modifiable

Significantly more parallel resources can be exploited with multigrid in time

- On massively parallel systems serial time integration becomes a bottleneck limiting the efficiency of simulations
- Parallel-in-time methods introduce an additional dimension of parallelism by distributing the workload in time across multiple processors

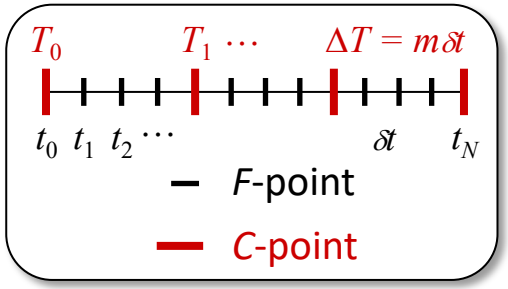


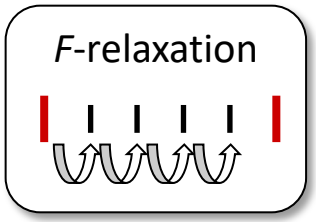


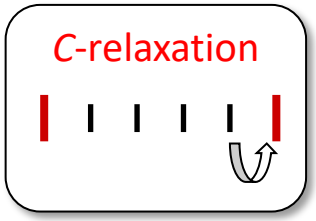
- Parallelize in space only
- Store only one time step
- Parallelize in space and time
- Store several time steps

Open source, flexible, and non-intrusive MGRIT implementation

- Create concurrency in the time dimension
- Non-intrusive with unchanged time discretization:
  - Converges to same solution as sequential stepping
  - Only stores *C*-points to minimize storage
  - Overlaps communication and computation
  - Extends to nonlinear problems with FAS formulation
- Speedups can be significant:
  - Useful only beyond some scale, there is a crossover point
  - Sometimes need significantly more parallelism just to break even
  - The more time steps, the more speedup potential
- **Allows for reuse of existing software**







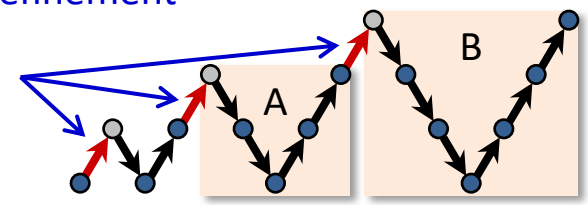
Relaxation alternates between *F* / *C*-points

- F-relax= integration over C intervals
- C-relax = one integration step

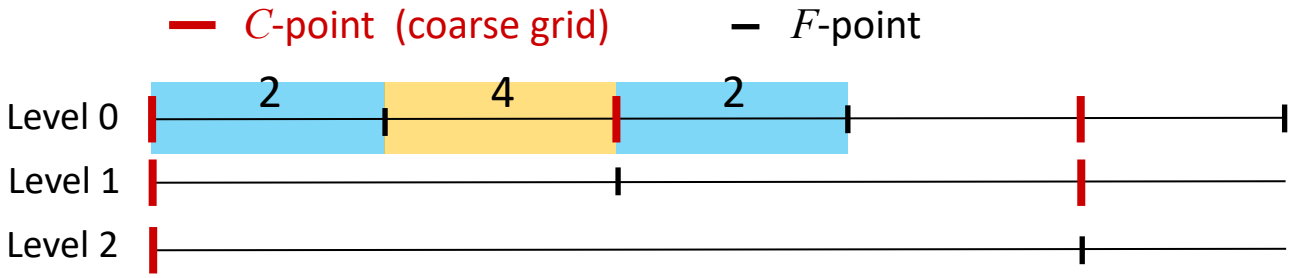
XBraid supports temporal adaptivity via an FMG-cycle

- User provides a refinement factor on the fine grid

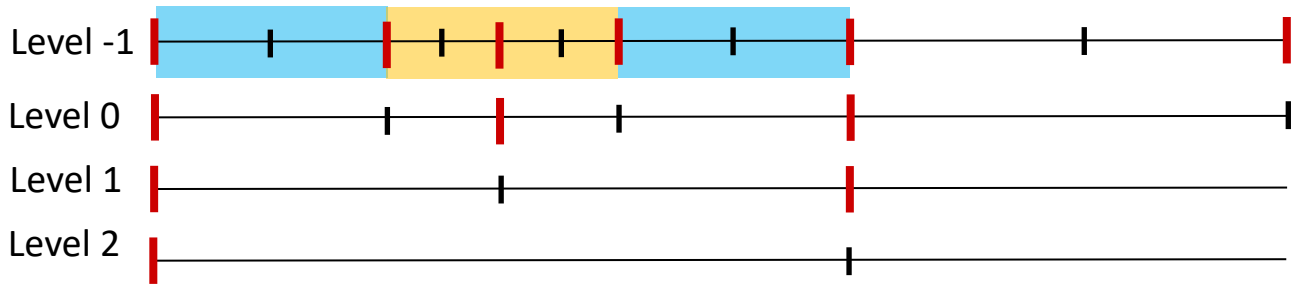
Temporal refinement done here



- Example time grid hierarchy (A)



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



Notice new C -pts

For more see Falgout et al. 2019

SUNDIALS + XBraid, what do we need?

- Two data structures:
  - An *App* structure holding any data needed by the interface
  - A *Vector* structure wrapping a SUNDIALS NVector
- Several wrapper functions:
  - Vector: *Clone, Free, Sum, SpatialNorm, and Buffer Size, Pack, and Unpack*
  - Other: *Init, Access, and Step*
- How much of the interfacing should the user supply and how much should be done by SUNDIALS? Goals:
  - Make things as simple as possible for a user that wants to try MGRIT
  - Provide as much flexibility as possible for the advanced user

SUNBraid: Vector Wrapper

```c
struct _braid_Vector_struct
{
  N_Vector y;
};

/* Poiner to vector wrapper (same as braid_Vector) */
typedef struct _braid_Vector_struct *SUNBraid_Vector;
```

```c
/* Compute alpha x + beta y -> y */
int SUNBraid_Vector_Sum(braid_App app,
                        braid_Real alpha, braid_Vector x,
                        braid_Real beta, braid_Vector y)
{
  N_VLinearSum(alpha, x->y, beta, y->y, y->y);
  return(0);
}
```

```c
/* Pack message buffer */
int SUNBraid_Vector_BufPack(braid_App app,
                            braid_Vector u, void *buffer,
                            braid_BufferStatus bstatus)
{
  int flag; /* return flag */

  /* Fill buffer */
  flag = N_VBufPack(u->y, buffer);
  if (flag != 0) return(1);

  return(0);
}
```

- Only a few small wrapper scripts are needed to use an NVector with XBraid
- Added new NVector buffer size, pack, and unpack functions:
  - N_VBufSize(v, size)
  - N_VBufPack(v, buf)
  - N_VBufUnpack(v, buf)
- Custom NVector modules only need to add these new functions to utilize the interface wrappers

SUNBraid: App Structure

```
/* Pointer to operations structure */
typedef struct _SUNBraidOps *SUNBraidOps;

/* Structure containing function pointers to operations */
struct _SUNBraidOps
{
  int (*init)(braid_App app, void *sun_mem, MPI_Comm comm_w,
              MPI_Comm comm_t, realtype tf, sunindextype nt,
              braid_Core *core);
  int (*free)(braid_App *app);
  int (*getudata)(braid_App app, void **user_data);
  int (*getvec)(braid_App app, N_Vector *y);
};

/* Define XBraid App structure */
struct _braid_App_struct
{
  void        *content;
  SUNBraidOps ops;
};

/* Pointer to the interface object (same as braid_App) */
typedef struct _braid_App_struct *SUNBraid_App;
```

- Generic SUNBraid_App structure follows the same object oriented design used for other SUNDIALS modules
- Individuals integrators or the user define the app content and implement the object operations
- This flexibly in defining the content makes it is easy to support simple uses case while accommodating advanced users

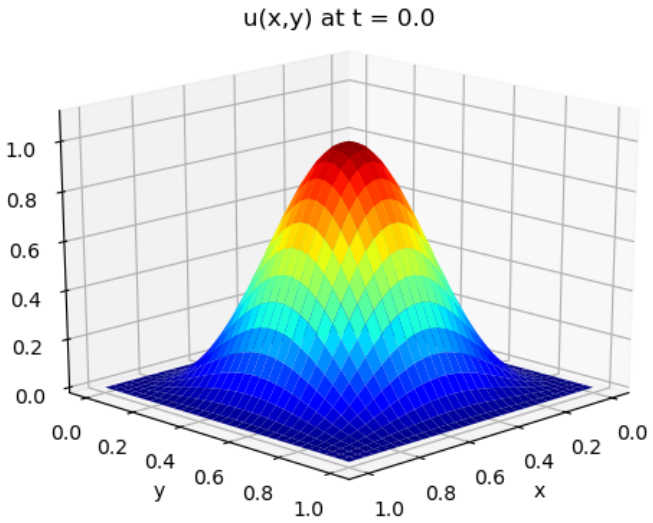
ARKBraid: App Structure

```
/* Define ARKode app content */
struct _ARKBraidAppContent
{
  /* ARKode memory structure */
  ARKodeMem ark_mem;

  /* Refinement options */
  booleantype refine;
  int max_refine;
  int rfactor_limit;

  /* Interface functions that a user may override */
  braid_PtFcnSpatialNorm spatialnorm;
  braid_PtFcnInit        init;
  braid_PtFcnAccess      access;
  braid_PtFcnStep        step;
};

typedef struct _ARKBraidAppContent *ARKBraidContent;
```

- The ARKode SUNBraid_App structure content holds
  - integrator memory,
  - optional parameters,
  - interface function pointers
- User setups the integrator as normal and attaches it with SUNBraidApp_Init(…)
- Set and Get functions allow users to modify or query most content

Example: 2D Heat Equation

- Problem setup:
  - Second order center differences in space
  - Second order SDIRK method in time
  - 128 x 128 mesh
  - MPI parallel in space
  - Inexact Newton with SUNDIALS PGC preconditioned using *hypre* PFMG
- Test Setups:
  - Fixed time stepping from [0, 1] with a step size of 1.0e-5
  - Adaptive time stepping from [0, 20] with various adaptivity controllers



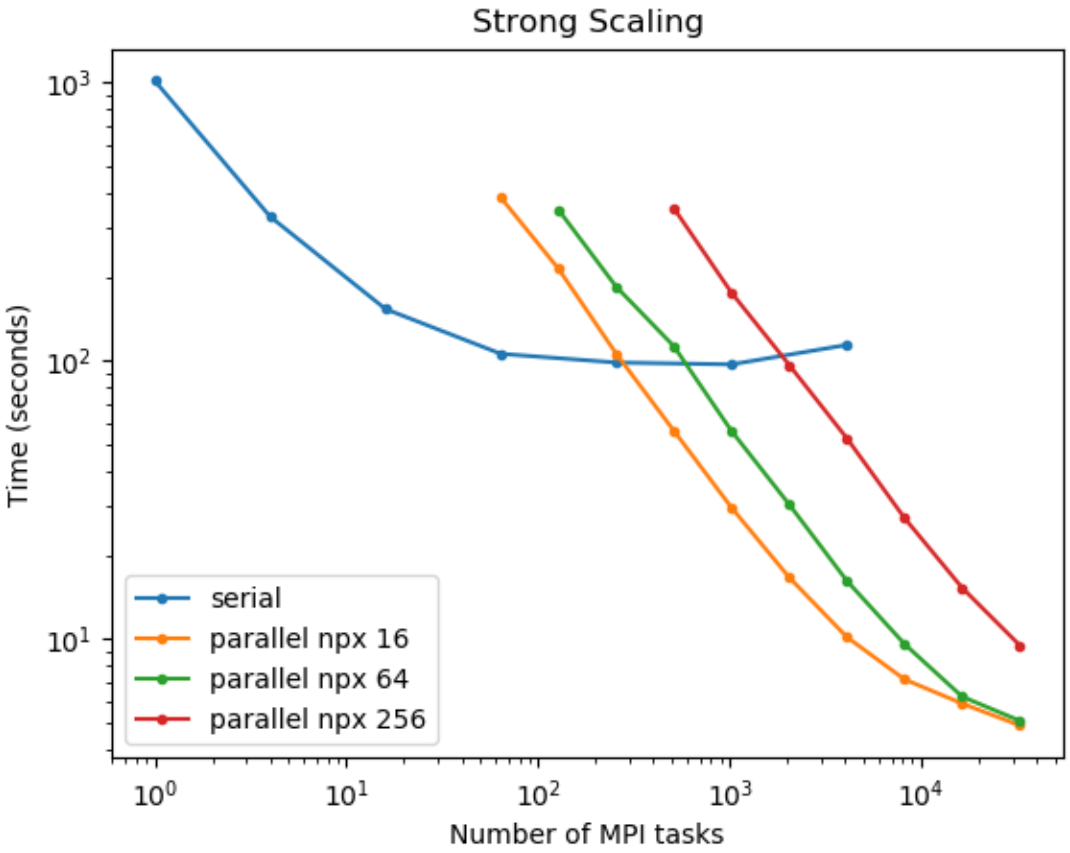
$$\frac{du}{dt} = \nabla^2 u + b(x, y, t)$$

The forcing term is chosen such that the analytic solution is

$$u(x, y, t) = \sin^2(\pi\, x) \sin^2(\pi\, y) \cos^2(\pi t)$$

Comparison of serial-in-time and parallel-in-time codes

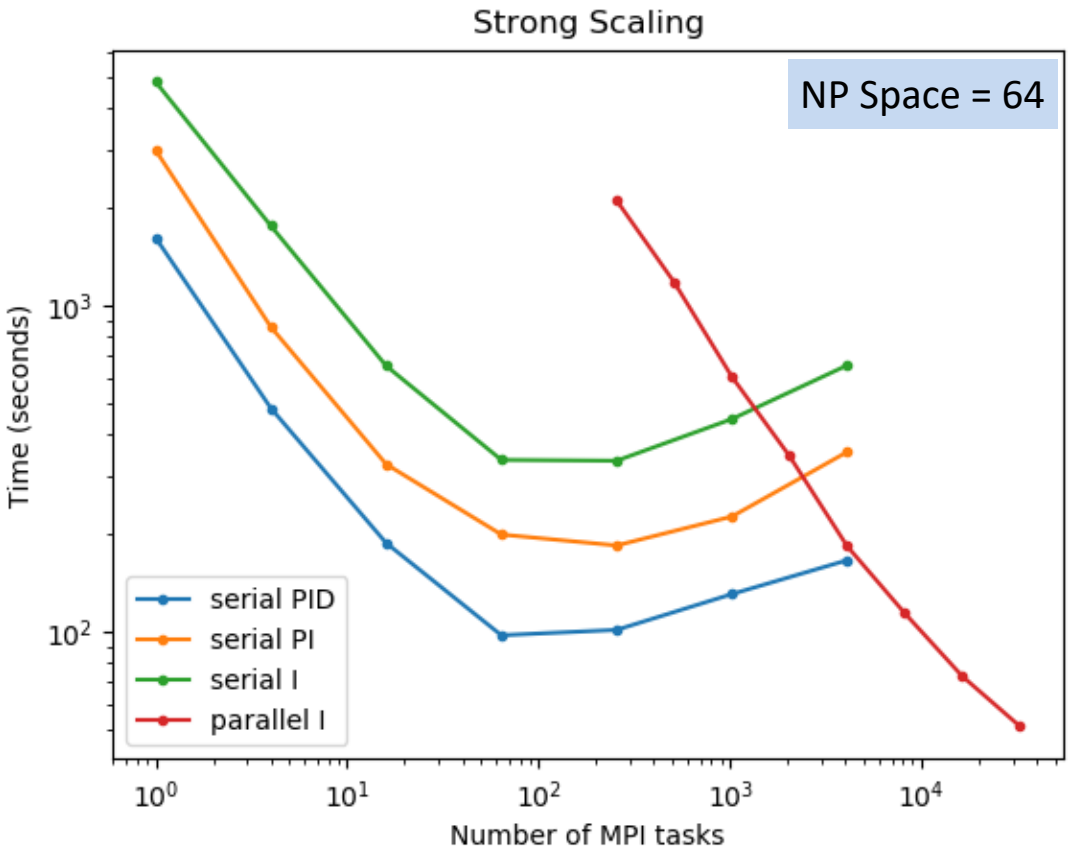
Example: 2D Heat Equation Fixed Step



NP Space	Speedup	Crossover
16	≈20x	≈256 (16)
64	≈20x	≈600 (10)
256	≈10x	≈1,024 (4)

- Setup:
  - Time interval [0, 1]
  - Step size 1.0e-5 s
  - Coarsening factors level 0 = 16, other levels = 2
  - ARKStep rtol = 10^{-4}, atol = 10^{-9}
  - Xbraid tol = $10^{-9}/\sqrt{dx * dy * dt}$
  - 2-norm in time and space

Example: 2D Heat Equation Adaptive Step



Controller	Speedup	Crossover
I	≈6.5x	≈256 (4)
PI	≈3.5x	≈4,096 (64)
PID	≈2x	≈10,000 (157)

Controller	Steps	Attempted
I	79,731	117,087
PI	51,285	62,109
PID	37,203	37,268
PinT (I)	63,263	--

- Setup: Time interval [0, 20], adaptive step sizes, coarsening factor 4 on all levels, ARKStep rtol = 10^{-4}, atol = 10^{-9}, Tol = $10^{-6}/\sqrt{dx * dy}$, max-norm in time, 2-norm in space

Takeaways and Current Work

- The non-intrusive design of the XBriad library makes it straight forward to interface with SUNDIALS' ARKode package
- MGRIT has shown potential for significant speedups by exposing parallelism in the time domain
- The SUNBraid interface requires minimal modification to existing code to get started and is flexible enough to accommodate advanced use cases

- Current work includes:
  - Exploring approaches for adapting solver tolerances and integrator parameters during the solve
  - Adding an option to supply a residual function to XBraid from SUNDIALS

- The XBraid interface will be release in SUNDIALS later this summer

Acknowledgements

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