Parallel-in-Time Optimization with the General-Purpose XBraid Package

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Outline

- Motivation: parallelizing optimization problems
- Parallel-in-time overview: Multigrid reduction in time (MGRIT)
- XBraid-adjoint code interface : Open source implementation
  - Non-intrusively uses existing user code
  - Example: user-interface for simple scalar ODE problem

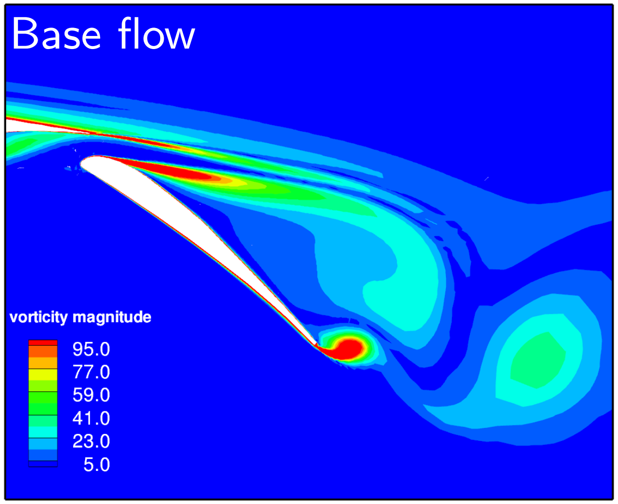
Motivation: PDE constrained optimization

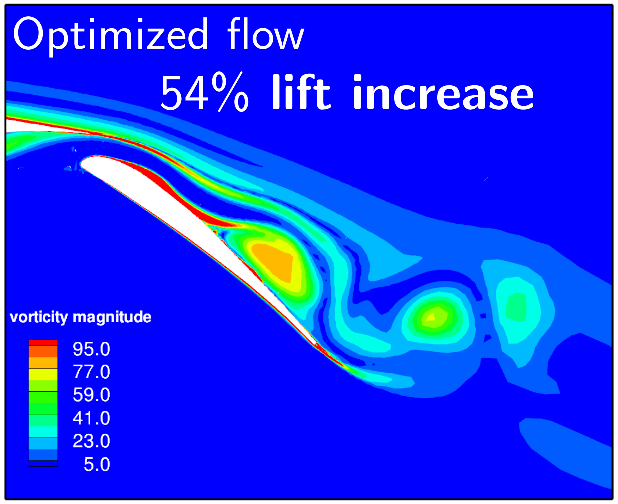
Example[1]

- Objective: Lift maximization
- Design: Amplitudes of actuation

Runtimes

- Simulation: 2.5h
- Optimization: 1,152h





1. Ötzkaya, Nemili et al., 2015

Problem description: Optimization with unsteady PDEs

- Optimize object function J, with a design variable u *(continuous)*

$$\min \frac{1}{T} \int_0^T J(y(t), u) dt$$

- While satisfying constraint of the forward in time process, with state variable y and initial condition g *(continuous)*

$$\frac{\delta y(t)}{\delta t} + c(y(t), u) = 0, \quad \forall t \in (0, T)$$

$$y(0) = g$$

Problem description: Optimization with unsteady PDEs

- Optimize object function J, with a design variable u *(discrete)*

$$\min \frac{1}{N} \sum_{i=1}^{N} J(y^i, u) \qquad J^n := J(y^n, u)$$

- While satisfying constraint of the forward in time process, with state variable y and initial condition g *(discrete)*

$$y^n = \Phi(y^{n-1}, u), \qquad n = 1, \ldots, N$$
$$y^0 = g$$

First Order Optimality Conditions

Form Lagrangian $L = \sum_{i}^{N} (J^n + (\bar{y}^n)^T (\Phi^{n-1} - y^n))$

1. State equations:

$$y^n = \Phi(y^{n-1}, u\ ), \qquad n = 1, \ldots, N$$
$$y^0 = g$$

2. Adjoint equations:

$$\bar{y}^n = \nabla_{y^n} J^n + (\delta_y \Phi^n)^T \bar{y}^n, \qquad n = N, \ldots, 1$$
$$\bar{y}^{N+1} = 0$$

3. Design equation:

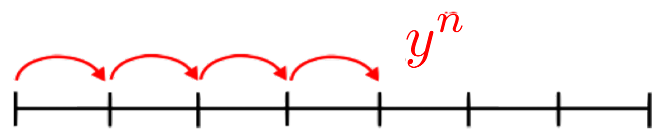
$$\sum_{n=1}^{N} \left(\nabla_u J^n + (\delta_u \Phi^{n-1})^T \bar{y}^{n-1}\right) = 0$$

Nested Optimization Approach

Initial design u_i

For $i = 1, 2, \ldots$

1. State equations **solve**:

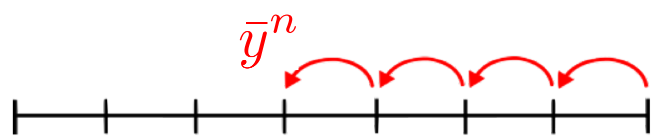


Time Parallel!

$$y^n = \Phi(y^{n-1}, u_i), \qquad n = 1, \ldots, N$$

$$y^0 = g$$

2. Adjoint equations **solve**:



Time Parallel!

$$\bar{y}^n = \nabla_{y^n} J^n + (\delta_y \Phi^n)^T \bar{y}^n, \qquad n = N, \ldots, 1$$

$$\bar{y}^{N+1} = 0$$

3. Design **update**:

$$u_{i+1} = u_i - B_i^{-1} \left(\sum_{n=1}^{N} (\nabla_u J^n + (\delta_u \Phi^{n-1})^T \bar{y}^n) \right)$$

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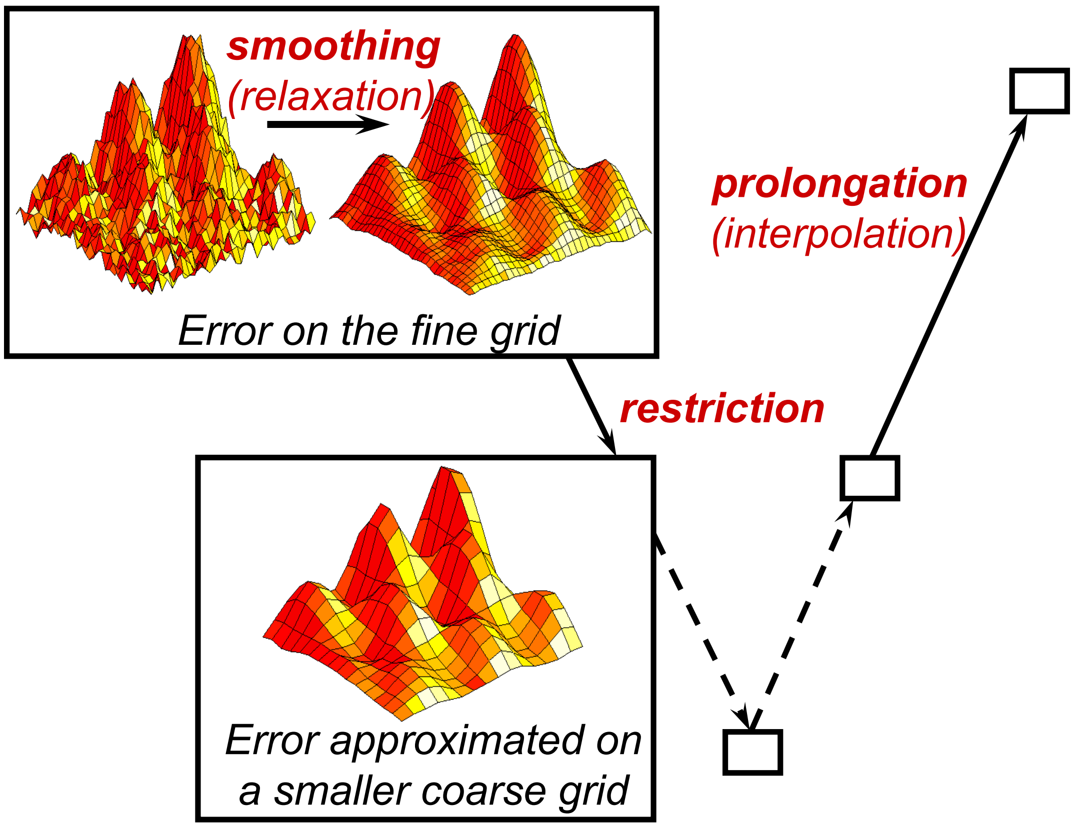
Parallel-in-time overview: Approach leverages spatial multigrid research

- **Motivation:** Clock speeds are stagnate but speedup still possible through more concurrency
  → Parallel-in-time is needed

The Multigrid V-cycle



Multigrid reduction in time (MGRIT)

- General one-step method for a **forward** evolution process

$$y^n = \Phi(y^{n-1}, u_i), \qquad n = 1, \ldots, N$$

- In the linear setting *(for simplicity)*, sequential marching $\equiv$ forward solve

$$A\mathbf{y} \equiv \begin{pmatrix} I & & & \\ -\Phi & I & & \\ & \ddots & \ddots & \\ & & -\Phi & I \end{pmatrix} \begin{pmatrix} y^0 \\ y^1 \\ \vdots \\ y^N \end{pmatrix} = \begin{pmatrix} g^0 \\ g^1 \\ \vdots \\ g^N \end{pmatrix} \equiv \mathbf{g}$$

- We solve this system **iteratively** with multigrid reduction *(MGR 1979)*
  - Replace sequential $O(N)$ method with $O(N)$ parallel alternative
  - Coarsens only in *time* → non-intrusive, i.e. Φ is "arbitrary"

Multigrid reduction in time (MGRIT)

- General one-step method for a **backward** evolution process

$$\bar{y}^n = \nabla_{y^n} J^n + (\delta_y \Phi^n)^T \bar{y}^n, \qquad n = N, \ldots, 1$$

- In the linear setting *(for simplicity)*, sequential marching $\equiv$ forward solve

$$\bar{A}\bar{\mathbf{y}} \equiv \begin{pmatrix} I & -\Phi^T & & & \\ & I & -\Phi^T & & \\ & & \ddots & \ddots & \\ & & & I & -\Phi^T \end{pmatrix} \begin{pmatrix} \bar{\boldsymbol{y}}^0 \\ \bar{\boldsymbol{y}}^1 \\ \vdots \\ \bar{\boldsymbol{y}}^N \end{pmatrix} = \begin{pmatrix} \nabla_{y^0} J^0 \\ \nabla_{y^1} J^1 \\ \vdots \\ \nabla_{y^N} J^N \end{pmatrix}$$

- We solve this system **iteratively** with multigrid reduction *(MGR 1979)*
  - Replace sequential $O(N)$ method with $O(N)$ parallel alternative
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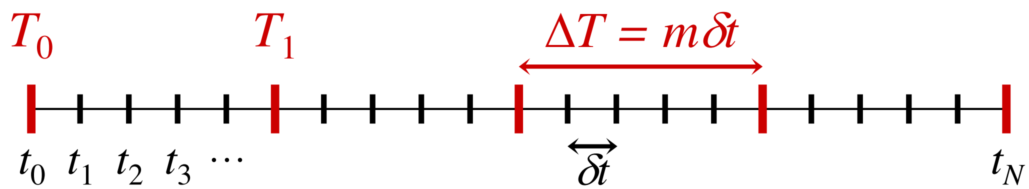
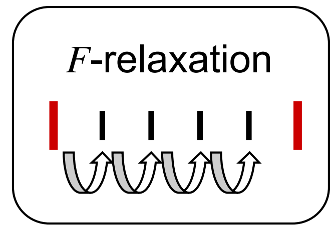
MGRIT for forward solve



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



- Relaxation is highly parallel
  - Alternates between F-points and C-points
  - F-relaxation = block Jacobi on each coarse time interval
- Coarse system approximates fine system
  - Approximate impractical Φ^m with Φ_Δ (e.g., time rediscretization with ΔT)

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

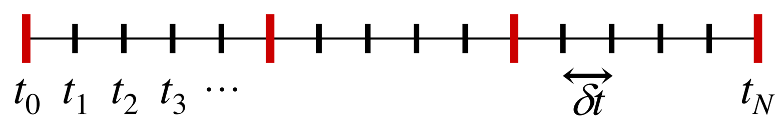
  - Apply recursively for multilevel hierarchy

A broader summary of MGRIT

- Expose **concurrency** in the evolution dimension with multigrid
- **Non-intrusive**, with unchanged fine-grid problem
- Converges to **same solution** as sequential marching

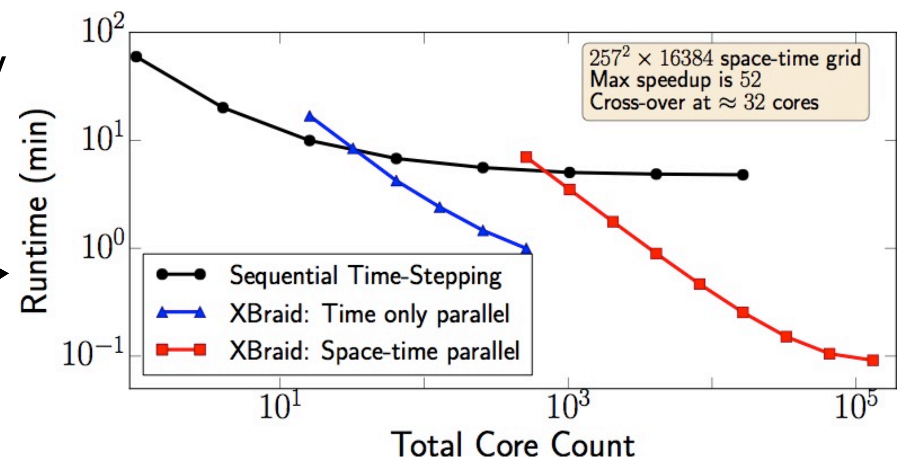
$$\begin{pmatrix} I & & & \\ -\Phi & I & & \\ & \ddots & \ddots & \\ & & -\Phi & I \end{pmatrix}$$

- Only store ***C*-points** to minimize storage
- Optimal for variety of parabolic problems
  - Converges in ~10 iterations for any coarsening factor



- Extends to **nonlinear** problems with FAS formulation
- In specialized two-level setting, MGRIT $\equiv$ Parareal

- Large speedups available, but in a new way
  - Time stepping is already O(N)
  - Useful only beyond a crossover
  - More time steps → more speedup potential
  - Example strong scaling of the 2D heat eqn →



- Much future work to do...

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XBraid-adjoint: open source & non-intrusive

- Solve for $\mathbf{y}, \ \bar{\mathbf{y}}, \ \bar{u} := (\delta J / \delta u)^T$ *(reduced gradient of J w.r.t. design u)*
- Wrap existing user code to obtain time parallelism

Standard XBraid: forward in time solve

1. **Step:** $y^n = \Phi(y^{n-1}, u)$
2. Clone
3. Sum: $y^m = \alpha y^n + \beta y^m$
4. SpatialNorm: $\|y^n\|$
5. Buf[Un]Pack
6. Init
7. Free
8. Access

Iteration k of XBraid:

$$\mathbf{y}_{k+1} \leftarrow \mathrm{XBraid}(\mathbf{y}_k, u_k)$$
$$J \leftarrow J(\mathbf{y}_k, u_k)$$

XBraid-adjoint: open source & non-intrusive

- Solve for $\mathbf{y}, \quad \bar{\mathbf{y}}, \quad \bar{u} := (\delta J/\delta u)^T$ *(reduced gradient of J w.r.t. design u)*
- Wrap existing user code to obtain time parallelism

XBraid-Adjoint

1. `ObjectiveT:` $J(y^n, u)$

2. `Step_diff:` $\bar{y}^n = (\delta_y \Phi^n)^T \bar{y}^{n+1}$

   $\bar{u} \mathrel{+}= (\delta_u \Phi^n)^T \bar{y}^{n+1}$

3. `ObjectiveT_diff:` $\bar{y}^n \mathrel{+}= \nabla_{y^n} J^n$

   $\bar{u} \mathrel{+}= \nabla_u J^n$

Iteration k of XBraid-adjoint:

$$\bar{\mathbf{y}}_{\mathbf{k+1}} \leftarrow \mathrm{XBraid\_adjoint}(\mathbf{y}_k, \bar{\mathbf{y}}_{\mathbf{k}}, u_k)$$

$$\bar{u} \leftarrow \frac{\delta J(\mathbf{y}_k, u_k)}{\delta u}$$

Functions 2 and 3 allow XBraid to compute

$$\bar{y}^n = \nabla_{y^n} J^n + (\delta_y \Phi^n)^T \bar{y}^{n+1}$$

$$u_{i+1} = u_i - B_i^{-1} \left(\sum_{n=1}^{N} (\nabla_u J^n + (\delta_u \Phi^{n-1})^T \bar{y}^n) \right)$$

Reduced gradient: $\bar{u}$

XBraid example: `ex-01-adjoint.c`

- Solve for the reduced gradient $\bar{u} := (\delta J / \delta u)^T$ *(later use in optimization)*
- Begin with simple problem: $J(y, \lambda) = 1/T \int_0^T \|y\| dt$

$$\text{s.t.} \qquad y_t = \lambda y$$
$$y(0) = 1$$

- First, user must define objects: `App` and `Vector`

```
typedef struct _braid_App_struct
{
   int         rank;
   double      design;
   double      gradient;

} my_App;

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

XBraid example: `ex-01-adjoint.c`

- `Step()`: $y^n = \Phi(y^{n-1}, u)$

```
int
my_Step(braid_App        app,
        braid_Vector     ystop,
        braid_Vector     fstop,
        braid_Vector     y,
        braid_StepStatus status)
{
```

...

```

   /* Get the design variable from the app */
   double lambda = app->design;

   /* Use backward Euler to propagate solution */
   (y->value) = 1./(1. - lambda * (tstop-tstart))*(y->value);

   return 0;
```

XBraid example: `ex-01-adjoint.c`

- `Step_diff()`: $\bar{y}^n = (\delta_y \Phi^n)^T \bar{y}^{n+1}$

  $$\bar{u} \mathrel{+}= (\delta_u \Phi^n)^T \bar{y}^{n+1}$$

```c
int
my_Step_diff(braid_App              app,
                braid_Vector        y,
                braid_Vector        y_bar,
                braid_StepStatus    status)
{
```

...

```c
   /* Get the design from the app */
   double lambda = app->design;

   /* Transposed derivative of step wrt y times y_bar */
   ddy = 1./(1. - lambda * deltat) * (y_bar->value);

   /* Transposed derivative of step wrt design times y_bar */
   ddesign = (deltat*(y->value)) / pow(1 - deltat*lambda,2) * (y_bar->value);

   /* Update y_bar and gradient */
   y_bar->value       = ddy;
   app->gradient     += ddesign;
```

XBraid example: `ex-01-adjoint.c`

- `ObjectiveT()` and `ObjectiveT_diff()` are similar
- Initialize and run XBraid-adjoint:

```
    /* Initialize XBraid */
    braid_Init( <insert function pointers> );

   /* Initialize adjoint-based gradient computation */
    braid_InitAdjoint( <insert function pointers> );
```

...

```
    braid_SetAbsTol(core, 1e-6);               /* Tolerance on state residual norm */
    braid_SetAbsTolAdjoint(core, 1e-6);        /* Tolerance on adjoint residual norm *


    /* Run simulation and adjoint-based gradient computation */
    braid_Drive(core);

    /* Get the objective function value from XBraid */
    braid_GetObjective(core, &objective);

    /* Collect sensitivities from all processors */
    double mygradient = app->gradient;
    MPI_Allreduce(&mygradient, &(app->gradient), 1, MPI_DOUBLE, MPI_SUM, comm);
```

$$\bar{u} \leftarrow (\delta J/\delta u)^T$$

XBraid example: `ex-01-adjoint.c`

- Run it!

```
schroder2@kullat:$ ./ex-01-adjoint

  Braid: Begin simulation, 50 time steps

  Braid:       || r ||       || r_adj ||      Objective
  Braid:---------------------------------------------
  Braid:    0  5.399995e-01  2.521756e-02  6.270806e-02
  Braid:    1  2.446737e-02  2.604047e-02  3.604351e-02
  Braid:    2  1.098316e-03  2.278004e-03  3.600016e-02
  Braid:    3  4.838178e-05  1.498949e-04  3.600000e-02
  Braid:    4  2.065806e-06  8.581917e-06  3.600000e-02
  Braid:    5  8.359592e-08  4.482596e-07  3.600000e-02

 Objective = 3.59999999999874e-02
 Gradient  = 1.92000799963229e-02
```

XBraid example: `ex-01-optimization.c`

- XBraid-adjoint solver
  - Generically solves adjoint equations, backwards in time
  - Generically computes reduced gradients $\bar{u}$
    → Designed to work with many optimization methods!

- Example: `ex-01-optimization.c`
  - Implements simple reduced space optimization loop
    (This is a template for implementing your favorite optimization method)
  - Requires:
    - Global objective evaluation function (and derivative)
    - Design update function
    - Halting metric (e.g., gradient norm)
  - Again, the goal is to wrap existing user code!

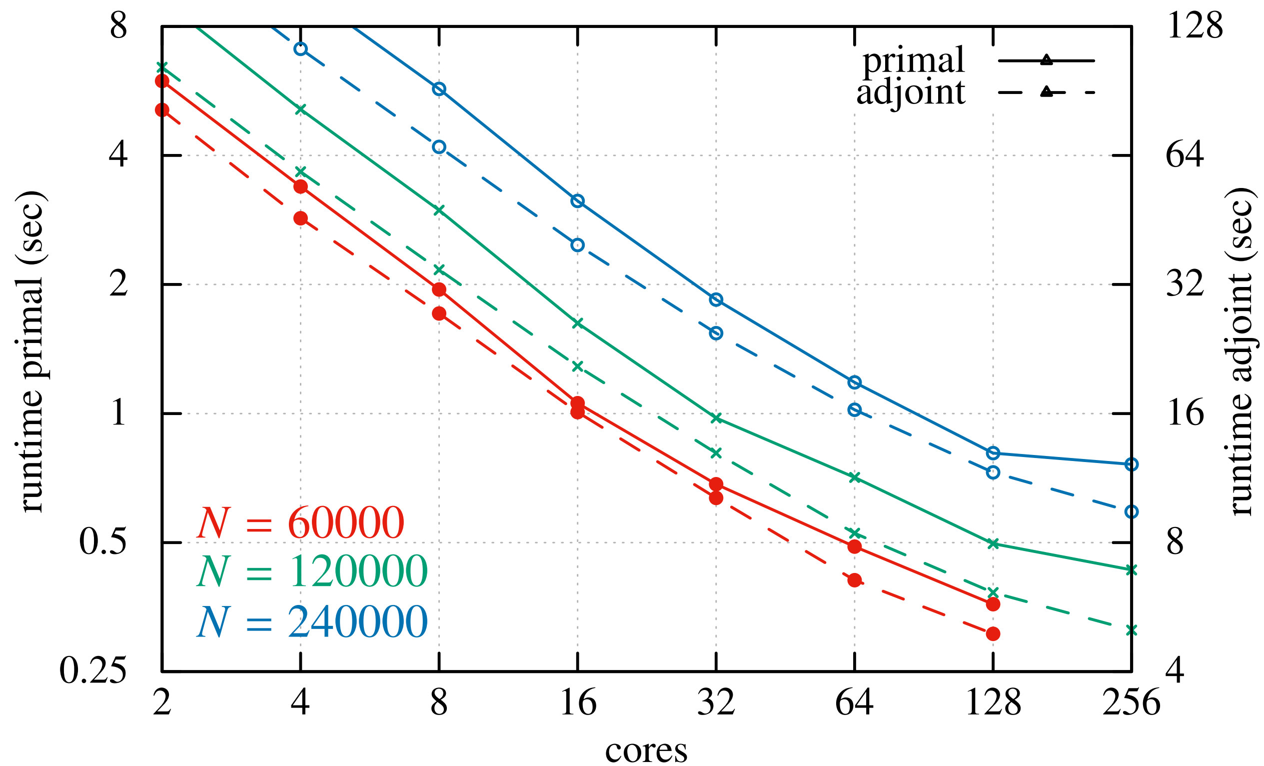
Model Problem: 1D advection-diffusion

- Advection dominated, with Van Der Pol oscillator on left boundary

$$y_t + y_x - \epsilon y_{xx} = 0, \quad \epsilon = 10^{-5}$$

- Tracking objective: Minimize difference of space-time averaged solution to preset value

- When used with one-shot strategies, the max speedup is 25x



Scaling of primal (solid lines) and adjoint (dashed lines) XBraid solvers.

Summary and Conclusions

- **Parallel time integration is needed** on future architectures, especially for adjoint-based optimization techniques

- **New XBraid-adjoint** non-intrusively couples with existing codes
  - Available in May, 2018 release
  - http://llnl.gov/casc/xbraid

- **References**

1. Günther, Gauger, and Schroder. *A Non-Intrusive Parallel-in-Time Approach for Simultaneous Optimization with Unsteady PDEs.* Optimization Methods and Software, (submitted), (2018).
2. Günther, Gauger, and Schroder. *A Non-Intrusive Parallel-in-Time Adjoint Solver with the XBraid Library.* CVS, Springer, (accepted), (2017).

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

XBRAID PARALLEL MULTIGRID IN TIME

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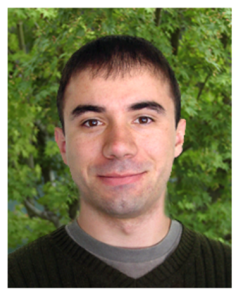
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Done