IMEX Methods in SUNDIALS: The ARKode Solver

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Outline

Outline

Multiphysics Problems

"Multiphysics problems" typically involve a variety of interacting processes:

- System of multiple components coupled in the bulk:
  - Cosmology: radiation + (magneto)hydrodynamics + chemistry + gravity
  - Combustion/subsurface flow: reaction + transport
- System of multiple components coupled across interfaces:
  - Climate: ocean + atmosphere + sea ice
  - Tokamak: fluid core + kinetic edge

In this talk, we'll consider the prototypical multiphysics form,

$$\partial_t u \;=\; f(t,u) \;=\; f_1(t,u) + f_2(t,u),$$

where u comprises all of our unknowns, and $f_i(t,u)$ are different physical processes that each act on all or part of u.

A primary difficulty with multiphysics problems is that each process may evolve at a different speed, e.g. $f_1(t,u)$ is "slow" while $f_2(t,u)$ is "fast".

Multiphysics Often Means "Multirate"

A single time scale is ideal for explicit-time methods, allowing for simpler algorithms, high-order accuracy, and predictable stability.

Wide temporal disparities can be analytically reformulated, but only for the scale of interest.

True multi-rate problems, however, require something more:

- Fully implicit methods are valid for stiff problems, but may require adaptation of solvers for all physical components.
- Operator-split methods are often chosen to match methods with physics.

Unfortunately, "standard" splitting approaches suffer from:

- *Low Accuracy* – even fractional-step methods may not achieve asymptotic $\mathcal{O}(h^2)$ accuracy until h is very small, since error terms are dominated by inter-process interactions [Ropp, Shadid,& Ober 2005].
- *Low Stability* – numerical stability isn't guaranteed *even if* h *is stable for each component* [Estep et al., 2007].

Fixing Operator Splitting

Although potentially dangerous, splittings are pervasive in scientific computing:

- Reuse existing/legacy software,
- Allow incorporation of domain-specific knowledge,
- No monolithic solvers for complex (and often non-differentiable) physics,
- Results "look reasonable," especially once the time stepping parameters have been tweaked.

Can we enhance splitting's stability & accuracy while retaining these benefits?

- The primary problem with basic splittings is that the component solvers are derived in isolation, with no concern for the coupling error.
- What if we instead derived new splitting approaches that explicitly account for inter-component coupling?

Outline

Additive Runge-Kutta Methods [Ascher et al. 1997; Araújo et al. 1997]

Although ARK methods may be derived for arbitrary splittings, here we consider splittings into two components: *explicit* and *implicit*,

$$\partial_t u = f_E(t,u) + f_I(t,u), \quad t \in [0,T], \quad u(0) = u_0,$$

We combine two s-stage methods (ERK + DIRK). Denoting $t_{n,j} = t_n + c_j h$,

$$z_i = u_n + h\sum_{j=1}^{i-1} a^E_{i,j} f_E(t_{n,j}, z_j) + h\sum_{j=1}^{i} a^I_{i,j} f_I(t_{n,j}, z_j), \quad i = 1,\ldots,s,$$

$$u_{n+1} = u_n + h\sum_{j=1}^{s} b_j \left(f_E(t_{n,j}, z_j) + f_I(t_{n,j}, z_j)\right) \quad \text{[solution]}$$

$$\tilde{u}_{n+1} = u_n + h\sum_{j=1}^{s} \tilde{b}^E_j \left(f_E(t_{n,j}, z_j) + f_I(t_{n,j}, z_j)\right) \quad \text{[embedding]}$$

We therefore have two Butcher tables to work with:

$$\begin{array}{c|cccc} c_1 & 0 & 0 & \cdots & 0 \\ c_2 & a^E_{2,1} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ c_s & a^E_{s,1} & \cdots & a^E_{s,s-1} & 0 \\ \hline & b_1 & \cdots & b_{s-1} & b_s \\ & \tilde{b}_1 & \cdots & \tilde{b}_{s-1} & \tilde{b}_s \end{array} \qquad \begin{array}{c|cccc} c_1 & a^I_{1,1} & 0 & \cdots & 0 \\ c_2 & a^I_{2,1} & a^I_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ c_s & a^I_{s,1} & \cdots & a^I_{s,s-1} & a^I_{s,s} \\ \hline & b_1 & \cdots & b_{s-1} & b_s \\ & \tilde{b}_1 & \cdots & \tilde{b}_{s-1} & \tilde{b}_s \end{array}$$

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ARK Coefficients

We have $s^2 + 3s$ total free parameters $\left(c_i, b_j, \tilde{b}_j, a^E_{i,j}, a^I_{i,j}\right)$. As with traditional RK methods, these are chosen to satisfy desired constraints:

- Maximize the order of accuracy for each elemental method,
- Maximize the stability of each elemental method,
- Simplify repeated implicit solves (e.g. SDIRK or ESDIRK),
- Enable accurate/stable embeddings for temporal error estimation,
- Conservation of certain integrals (linear & quadratic first integrals).

Additionally, ARK methods must also satisfy coupling conditions *between* the methods, to the same accuracy as each elemental method.

ARK Solution Algorithm – Tables

To better understand the workings of an ARK time step, let's consider the ERK/ESDIRK pair, ARK3(2)4L[2]SA [Kennedy & Carpenter, 2001],

0	0	0	0	0
0.87	0.87	0	0	0
0.6	0.53	0.07	0	0
1.0	0.40	-0.44	1.04	0
	0.19	-0.60	0.97	0.44
	0.21	-0.49	0.87	0.40

0	0	0	0	0
0.87	0.44	0.44	0	0
0.6	0.26	-0.09	0.44	0
1.0	0.19	-0.60	0.97	0.44
	0.19	-0.60	0.97	0.44
	0.21	-0.49	0.87	0.40

ARK Solution Algorithm – Stage 1

To better understand the workings of an ARK time step, let's consider the ERK/ESDIRK pair, ARK3(2)4L[2]SA [Kennedy & Carpenter, 2001],

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 0.87 & 0.87 & 0 & 0 & 0 \\ 0.6 & 0.53 & 0.07 & 0 & 0 \\ 1.0 & 0.40 & -0.44 & 1.04 & 0 \\ \hline & 0.19 & -0.60 & 0.97 & 0.44 \\ & 0.21 & -0.49 & 0.87 & 0.40 \end{array} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 0.87 & 0.44 & 0.44 & 0 & 0 \\ 0.6 & 0.26 & -0.09 & 0.44 & 0 \\ 1.0 & 0.19 & -0.60 & 0.97 & 0.44 \\ \hline & 0.19 & -0.60 & 0.97 & 0.44 \\ & 0.21 & -0.49 & 0.87 & 0.40 \end{array}$$

Stage 1: $z_1 = u_n$,

ARK Solution Algorithm – Stage 2

To better understand the workings of an ARK time step, let's consider the ERK/ESDIRK pair, ARK3(2)4L[2]SA [Kennedy & Carpenter, 2001],

0	0	0	0	0
0.87	0.87	0	0	0
0.6	0.53	0.07	0	0
1.0	0.40	−0.44	1.04	0
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	0.21	−0.49	0.87	0.40

0	0	0	0	0
0.87	0.44	0.44	0	0
0.6	0.26	−0.09	0.44	0
1.0	0.19	−0.60	0.97	0.44
	0.19	−0.60	0.97	0.44
	0.21	−0.49	0.87	0.40

Stage 1: $z_1 = u_n,$

Stage 2: $z_2 - 0.44 h f_I(t_{n,2}, z_2) = u_n + h\left(a^E_{2,1} f_E(t_{n,1}, z_1) + a^I_{2,1} f_I(t_{n,1}, z_1)\right),$

ARK Solution Algorithm – Stage 3

To better understand the workings of an ARK time step, let's consider the ERK/ESDIRK pair, ARK3(2)4L[2]SA [Kennedy & Carpenter, 2001],

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 0.87 & 0.87 & 0 & 0 & 0 \\ 0.6 & 0.53 & 0.07 & 0 & 0 \\ 1.0 & 0.40 & -0.44 & 1.04 & 0 \\ \hline & 0.19 & -0.60 & 0.97 & 0.44 \\ & 0.21 & -0.49 & 0.87 & 0.40 \end{array} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 0.87 & 0.44 & 0.44 & 0 & 0 \\ 0.6 & 0.26 & -0.09 & 0.44 & 0 \\ 1.0 & 0.19 & -0.60 & 0.97 & 0.44 \\ \hline & 0.19 & -0.60 & 0.97 & 0.44 \\ & 0.21 & -0.49 & 0.87 & 0.40 \end{array}$$

Stage 1: $z_1 = u_n,$

Stage 2: $z_2 - 0.44 h f_I(t_{n,2}, z_2) = u_n + h \left(a^E_{2,1} f_E(t_{n,1}, z_1) + a^I_{2,1} f_I(t_{n,1}, z_1) \right),$

Stage 3: $z_3 - 0.44 h f_I(t_{n,3}, z_3) = u_n + h \sum_{j=1}^{2} \left(a^E_{3,j} f_E(t_{n,j}, z_j) + a^I_{3,j} f_I(t_{n,j}, z_j) \right),$

ARK Solution Algorithm – Stage 4

To better understand the workings of an ARK time step, let's consider the ERK/ESDIRK pair, ARK3(2)4L[2]SA [Kennedy & Carpenter, 2001],

0	0	0	0	0
0.87	0.87	0	0	0
0.6	0.53	0.07	0	0
1.0	0.40	−0.44	1.04	0
	0.19	−0.60	0.97	0.44
	0.21	−0.49	0.87	0.40

0	0	0	0	0
0.87	0.44	0.44	0	0
0.6	0.26	−0.09	0.44	0
1.0	0.19	−0.60	0.97	0.44
	0.19	−0.60	0.97	0.44
	0.21	−0.49	0.87	0.40

Stage 1: $z_1 = u_n,$

Stage 2: $z_2 - 0.44hf_I(t_{n,2}, z_2) = u_n + h\left(a^E_{2,1} f_E(t_{n,1}, z_1) + a^I_{2,1} f_I(t_{n,1}, z_1)\right),$

Stage 3: $z_3 - 0.44hf_I(t_{n,3}, z_3) = u_n + h\sum_{j=1}^{2}\left(a^E_{3,j} f_E(t_{n,j}, z_j) + a^I_{3,j} f_I(t_{n,j}, z_j)\right),$

Stage 4: $z_4 - 0.44hf_I(t_{n,4}, z_4) = u_n + h\sum_{j=1}^{3}\left(a^E_{4,j} f_E(t_{n,j}, z_j) + a^I_{4,j} f_I(t_{n,j}, z_j)\right),$

ARK Solution Algorithm – Finish

To better understand the workings of an ARK time step, let's consider the ERK/ESDIRK pair, ARK3(2)4L[2]SA [Kennedy & Carpenter, 2001],

0	0	0	0	0
0.87	0.87	0	0	0
0.6	0.53	0.07	0	0
1.0	0.40	−0.44	1.04	0
	0.19	−0.60	0.97	0.44
	0.21	−0.49	0.87	0.40

0	0	0	0	0
0.87	0.44	0.44	0	0
0.6	0.26	−0.09	0.44	0
1.0	0.19	−0.60	0.97	0.44
	0.19	−0.60	0.97	0.44
	0.21	−0.49	0.87	0.40

Stage 1: $z_1 = u_n,$

Stage 2: $z_2 - 0.44hf_I(t_{n,2}, z_2) = u_n + h\left(a^E_{2,1} f_E(t_{n,1}, z_1) + a^I_{2,1} f_I(t_{n,1}, z_1)\right),$

Stage 3: $z_3 - 0.44hf_I(t_{n,3}, z_3) = u_n + h\sum_{j=1}^{2}\left(a^E_{3,j} f_E(t_{n,j}, z_j) + a^I_{3,j} f_I(t_{n,j}, z_j)\right),$

Stage 4: $z_4 - 0.44hf_I(t_{n,4}, z_4) = u_n + h\sum_{j=1}^{3}\left(a^E_{4,j} f_E(t_{n,j}, z_j) + a^I_{4,j} f_I(t_{n,j}, z_j)\right),$

Finish: $u_{n+1} = u_n + h\sum_{j=1}^{4} b_j\left(f_{E,j} + f_{I,j}\right)$ and $\tilde{u} = u_n + h\sum_{j=1}^{4} \tilde{b}_j\left(f_{E,j} + f_{I,j}\right).$

ARK Algorithm Comments

Key algorithm characteristics:

- f_E components relegated to RHS, implicit solvers treat only f_I.
- Three implicit solves – all are nearly identical but with differing RHS.
  - If f_I is linear and independent of t, the LHS are in fact identical, and stages may reuse matrices and solvers.
  - Even if nonlinear or time-dependent, costly analytical Jacobians and factorizations may be reused for preconditioning.
- Implicit method is A-stable, L-stable and stiffly accurate.
- u_{n+1} is globally $\mathcal{O}(h^3)$ accurate; $\tilde{u}$ is $\mathcal{O}(h^2)$; z_i are $\mathcal{O}(h^2)$.
- Since IRK portion is A-stable, linear instability can only arise due to the ERK, so time steps must satisfy the explicit stability restriction,

$$h \leq h_{exp},$$

otherwise may be chosen to track a desired accuracy via $\|u_{n+1} - \tilde{u}\|$.

The ARKode Library

As a part of the FASTMath SciDAC Institute, we are constructing a library comprising these solvers named *ARKode*, that will be released as a new component solver within SUNDIALS.

- Nearly identical user interface as CVODE, albeit with separate user-specified $f_E(t, y)$ and $f_I(t, y)$ routines.
- Data structure agnostic – as long as the basic vector kernels are supplied this works with your native data structures.
- High-order accurate dense output, allowing efficient interpolation of results between integration steps, and reliable implicit predictors.
- Parameters optimized for iterative solvers and large-scale parallelism.
- Exhaustive suite of example and regression test problems.

The ARKode Library

Key differences between ARKode and CVODE include:

- Support for disabling either f_E or f_I, allowing adaptive DIRK or ERK.
- Optional accelerated fixed-point nonlinear solver,
- Optional PCG, FGMRES Krylov solvers,
- Support for non-identity mass matrix, $Mu' = f_E(t,u) + f_I(t,u)$,
- "Hot restart" support for problems with spatial adaptivity.
- "Set routines" allowing complete control over: Butcher table coefficients, time step adaptivity algorithm, temporal error estimation algorithm, implicit predictor algorithm, all internal solver parameters.

Plans:

- Fall 2013 public release; "friendly-user" release available now.
- Future support for partitioned symplectic methods (Hamiltonian systems).

Transitioning Between CVODE and ARKode

Consistent API simplifies experimentation:

```
#include <cvode/cvode.h>
#include <cvode/cvode_dense.h>
#include <sundials/sundials_types.h>



/* User-supplied Functions */
static int f(realtype t, N_Vector y,
             N_Vector ydot, void *udata);
static int Jac(long int N, realtype t, N_Vector y,
               N_Vector fy, DlsMat J, void *udata,
               N_Vector t1, N_Vector t2, N_Vector t3);

int main() {

   ...

  void *cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
  CVodeInit(cvode_mem, f, T0, y);
  CVodeSStolerances(cvode_mem, reltol, abstol);
  CVDense(cvode_mem, NEQ);
  CVDlsSetDenseJacFn(cvode_mem, Jac);

  for (iout=0; iout<Nt; iout++)
    CVode(cvode_mem, tout, y, &t, CV_NORMAL);
}
```

```
#include <arkode/arkode.h>
#include <arkode/arkode_dense.h>
#include <sundials/sundials_types.h>

/* User-supplied Functions */
static int fe(realtype t, N_Vector y,
              N_Vector ydot, void *udata);
static int fi(realtype t, N_Vector y,
              N_Vector ydot, void *udata);
static int Jac(long int N, realtype t, N_Vector y,
               N_Vector fy, DlsMat J, void *udata,
               N_Vector t1, N_Vector t2, N_Vector t3);

int main() {

   ...

  void *arkode_mem = ARKodeCreate();
  ARKodeInit(arkode_mem, fe, fi, T0, y);
  ARKodeSStolerances(arkode_mem, reltol, abstol);
  ARKDense(arkode_mem, NEQ);
  ARKDlsSetDenseJacFn(arkode_mem, Jac);

  for (iout=0; iout<Nt; iout++)
    ARKode(arkode_mem, tout, y, &t, ARK_NORMAL);
}
```

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Outline

PDE Cosmology Model Problem – Radiating Ionization Front

Find $u(\mathbf{x},t)$, $v(\mathbf{x},t)$ s.t. for $(\mathbf{x},t) \in [-1,1]^3 \times [0,1]$,

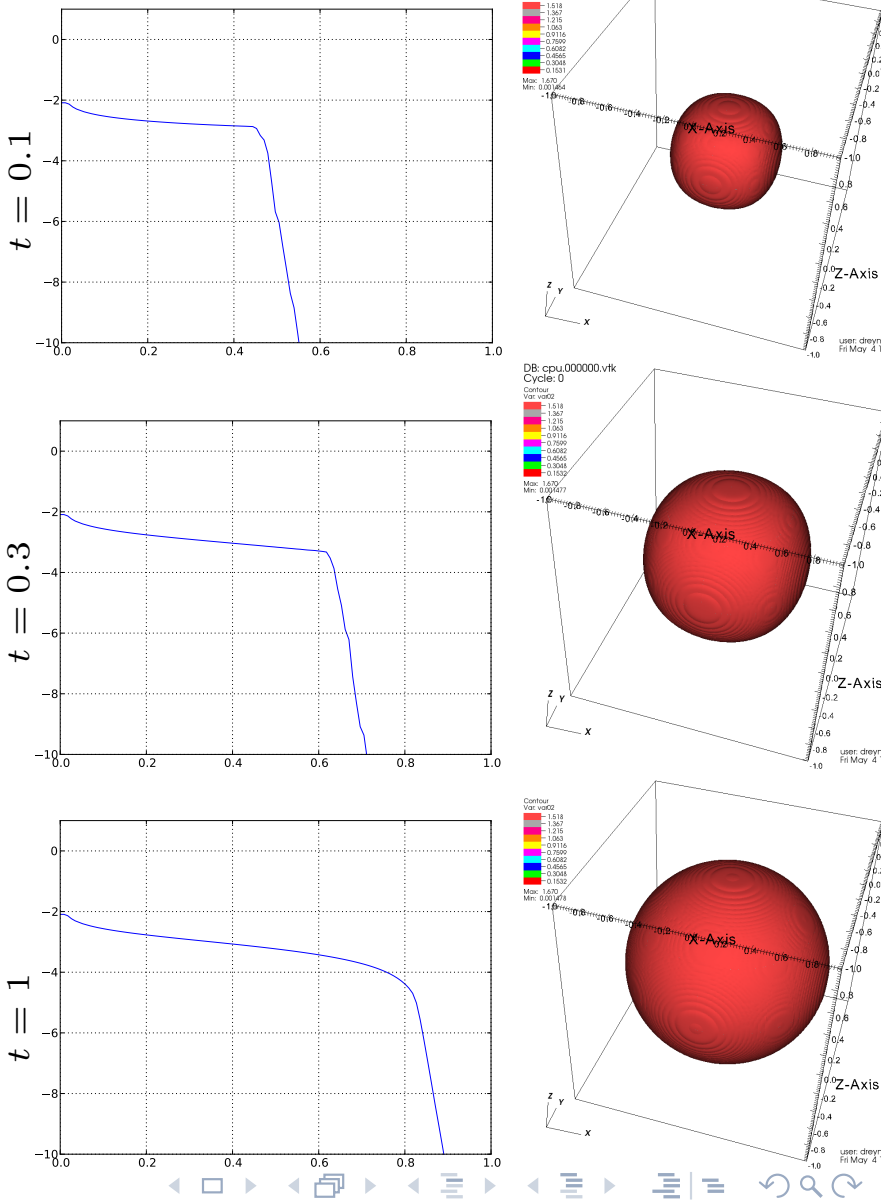
$$\begin{aligned} \partial_t u &= \nabla \cdot (\beta u) + \nabla \cdot (\mu \nabla u) + f_u(u,v), \\ \partial_t v &= \nabla \cdot (\beta v) + f_v(u,v), \end{aligned}$$

Where

- $u(\mathbf{x},0) = 10^{-8}, \quad v(\mathbf{x},0) = 1.67.$
- $\nabla u \cdot \mathbf{n}|_{\partial\Omega} = 0, \quad \nabla v \cdot \mathbf{n}|_{\partial\Omega} = 0.$
- $f_u(u,v) = 25000\,\delta_0(\mathbf{x}) - 1800000\,uv.$
- $f_v(u,v) = a(c-v)^2 - bv(c-v) + 567000\,uv.$
- $\beta(u,v,\mathbf{x}) = -\frac{\alpha u(c-v)}{\|\mathbf{x}\|}\mathbf{x}, \quad \alpha = \{10, 100, 250\},$
- $\mu(v) = \frac{100}{v},$
- $a = 2.445, \quad b = 0.01118, \quad c = 1.673.$

$\log_{10}(u)$ Profiles

Ionized region



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Radiating Ionization Test Solvers

Discretizations:

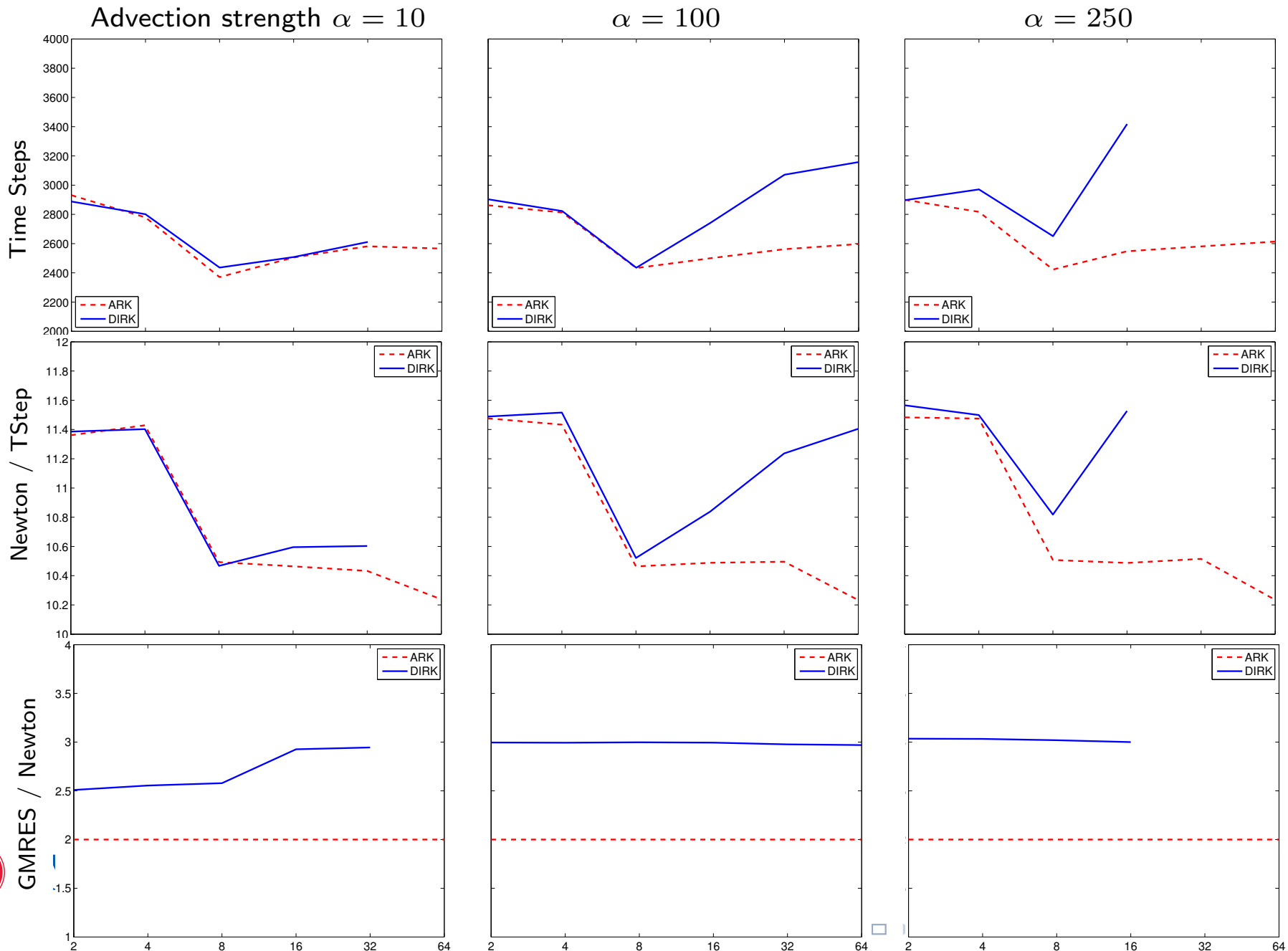
- FV grid of size $N_x \times N_y \times N_z$, with a fixed $32 \times 32 \times 32$ grid per MPI task.
- Process sizes: 2(2x1x1), 4(2x2x1), 8(2x2x2), 16(4x2x2), 32(4x4x2), 64(4x4x4).
- $\nabla \cdot (\mu \nabla u)$ discretized using 2nd-order centered differences.
- $\nabla \cdot (\beta u)$ discretized using CD or $\mathcal{O}(\triangle \mathrm{x})$ upwind, depending on $\|\beta\| > 10^{-3}$.
- Time: $\mathcal{O}(\Delta t^4)$ ARK and DIRK methods.

Solvers:

- Nonlinear: inexact Newton, `maxit` $= 5$.
- Linear: matrix-free GMRES, `maxit` $= 50$.
- Precond: AMG [HYPRE], Rx-Diff only (no advection).
- PID controller [Kennedy & Carpenter, 2001], with error estimate

$$e = \left(\frac{1}{N} \sum_i \left(\frac{u_i - \tilde{u}_i}{r_{tol} u_i + a_{tol}} \right)^2 \right)^{1/2}, \quad r_{tol} = 10^{-3}, \quad a_{tol} = 10^{-9}.$$

Radiating Ionization Results – Iteration Weak Scaling



Outline

Conclusions

ARK methods allow accurate/stable splitting of multi-rate problems:

- IMEX couplings are properly handled,
- No Dahlquist barrier – high accuracy and stability simultaneously possible.

RK under-pinnings allow robust and theoretically rigorous methods for error estimation and time adaptivity.

Works well with spatial adaptivity (due to one-step approach), with tunings for vector resizing and finite element discretizations.

Flexible infrastructure:

- Allows adaptive ERK or IRK methods alone,
- Enables domain-specific knowledge into the formulation.

"Convenient" preconditioners need not be chastised, since many solver difficulties (non-differentiability, nonlinearity, complex discretizations) often lie in slow components that can be treated explicitly.

Thanks & Acknowledgements

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- Carol S. Woodward [LLNL]
- Alan C. Hindmarsh [LLNL]
- David J. Gardner [SMU, PhD]
- Jean M. Sexton [SMU, MS]

Current Grant/Computing Support:

- DOE SciDAC & INCITE Programs
- NSF AST & XSEDE Programs
- DOD DURIP Program
- SMU Center for Scientific Computation

Software:

- ARKode – `http://faculty.smu.edu/reynolds/arkode`
- SUNDIALS – `https://computation.llnl.gov/casc/sundials`
- Enzo (cosmology) – `http://enzo-project.org`

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First-Order Splittings

Denote $S_i(h, u(t_n))$ as a solver for the component $\partial_t u = f_i(t, u)$ over a time step $t_n \to t_n + h \equiv t_{n+1}$, with initial condition $u(t_n)$.

To evolve $u(t_n) \to u(t_{n+1})$, we can use different solvers at the same h,

$$\begin{aligned} \hat{u} &= S_1\left(h, u(t_n)\right), \\ u(t_{n+1}) &= S_2\left(h, \hat{u}\right), \end{aligned}$$

or we may subcycle time steps for individual components,

$$\begin{aligned} \hat{u}_{j+1} &= S_1\left(\tfrac{h}{m}, \hat{u}_j\right),\ j = 0, \ldots, m, \quad \hat{u}_0 = u(t_n), \\ u(t_{n+1}) &= S_2\left(h, \hat{u}_m\right), \end{aligned}$$

Unless the S_i commute [i.e. $S_1(h, S_2(h, u)) = S_2(h, S_1(h, u))$] or the splitting is symmetric, these methods are at best $O(h)$ accurate *(no matter the accuracy of the individual solvers)*.

Fractional Step (Strang) Splitting [Strang 1968]

"Strang splitting" attempts to achieve a higher-order method using these separate component solvers, through manually symmetrizing the operator:

$$\hat{u}_1 = S_1\left(\tfrac{h}{2}, u(t_n)\right),$$

$$\hat{u}_2 = S_2\left(h, \hat{u}_1\right),$$

$$u(t_{n+1}) = S_1\left(\tfrac{h}{2}, \hat{u}_2\right).$$

This approach is $O(h^2)$ as long as each S_i is $O(h^2)$.

However:

- This asymptotic accuracy may not be achieved until h is very small, since error terms are dominated by inter-process interactions [Ropp, Shadid,& Ober 2005].
- Numerical stability isn't guaranteed *even if* h *is stable for each component* [Estep et al., 2007].

Operator-Splitting Issues – Accuracy [Ropp, Shadid, & Ober 2005]

Coupled systems can admit destabilizing modes not present in either component, due to *numerical resonance instabilities* [Grubmüller 1991].

Brusselator Example (Reaction-Diffusion):

$$\partial_t T = \tfrac{1}{40}\nabla^2 T + 0.6 - 3T + T^2 C,$$
$$\partial_t C = \tfrac{1}{40}\nabla^2 C + 2T - T^2 C,$$

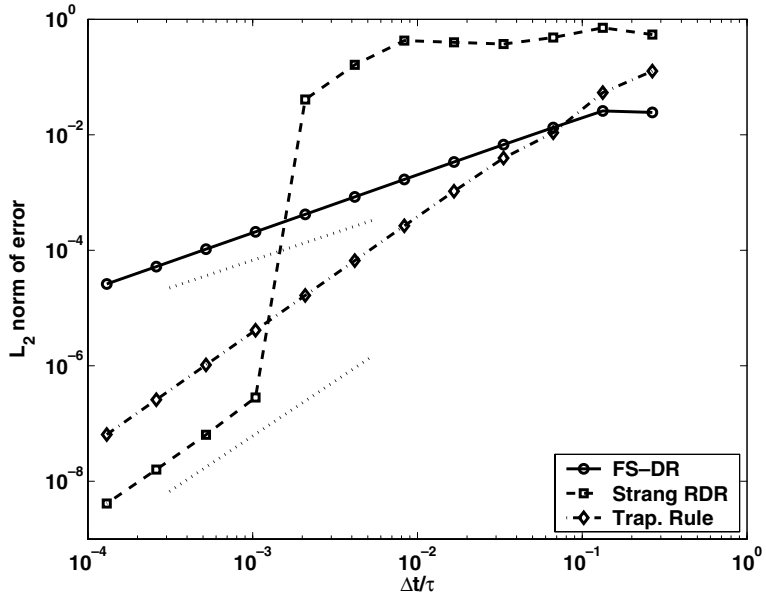
Three solvers:

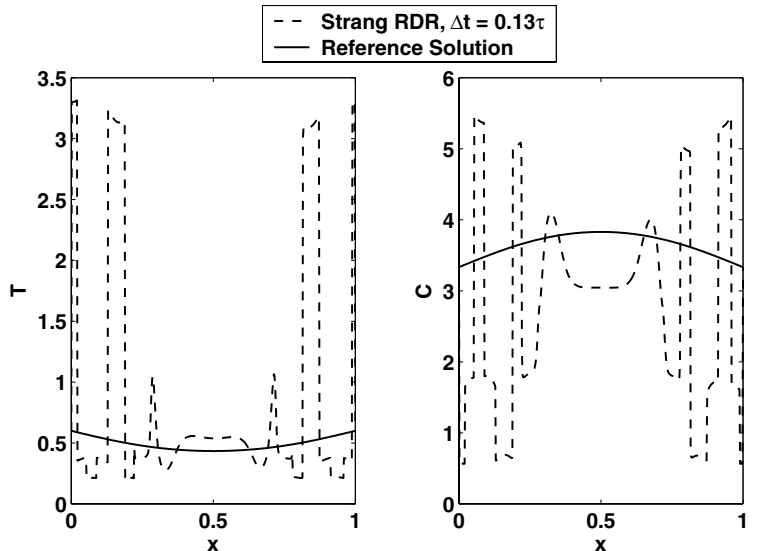
(a) Basic split: D (trap.) then R (subcycled BDF).

(b) Strang: $\frac{h}{2}$R, hD, $\frac{h}{2}$R,

(c) Fully implicit trapezoidal rule,

Results:
(a) is stable but inaccurate for all tests;
(b) unusable until h is "small enough".





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Operator Splitting Issues – Accuracy [Estep 2007]

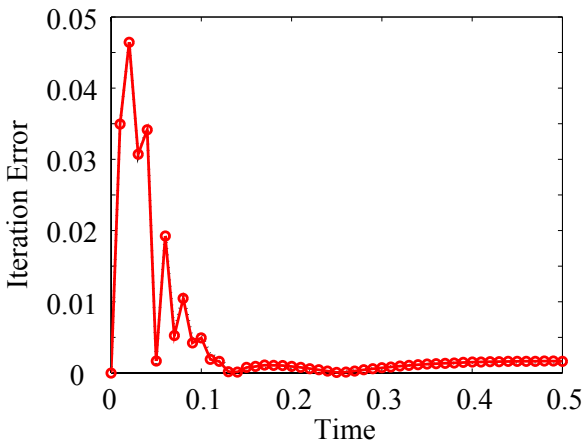
Consider $\Omega = \Omega_1 \cup \Omega_2$ where the subdomains share a boundary $\Gamma = \partial\Omega_1 \cap \partial\Omega_2$:

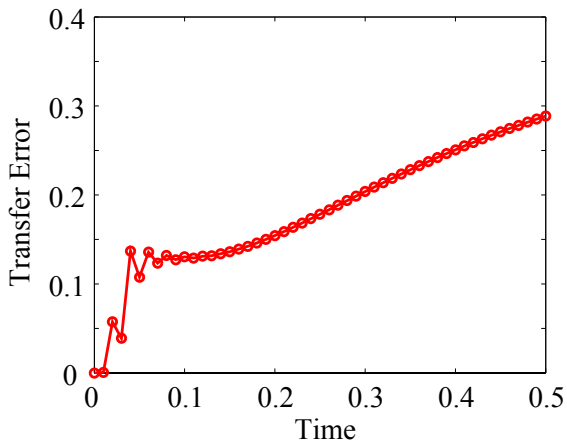
$$\partial_t u_1 = \nabla^2 u_1, \; x \in \Omega_1, \qquad \partial_t u_2 = \tfrac{1}{2}\nabla^2 u_2, \; x \in \Omega_2,$$

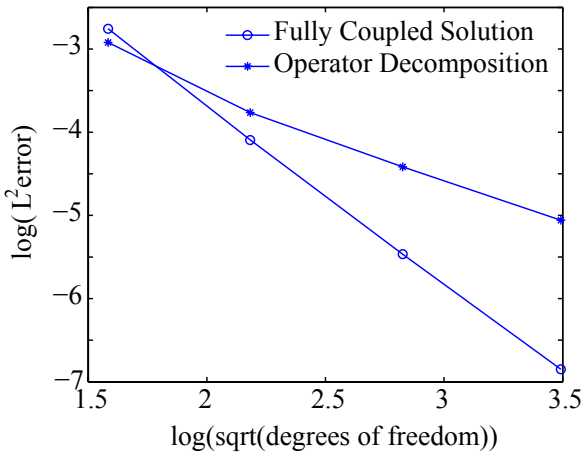
$$u_1 = u_2, \qquad \nabla u_1 \cdot n = \nabla u_2 \cdot n, \qquad \text{for } x \in \Gamma.$$

Solved using one Gauss-Seidel iteration: S_1 on Ω_1, then S_2 on Ω_2 (both trapezoidal). Errors from not iterating to convergence, and from error transfer between subdomains.

Using adjoints, they measured these errors separately:







- Error from incomplete iteration decreased with time.
- Transfer error accumulated and became dominant with time.
- While each S_i was $O(h^2)$, the coupled method was only $O(h)$.

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Operator-Splitting Issues – Stability [Estep et al., 2007]

Second Reaction-Diffusion Example (split subcycling; exact solvers):

$$\partial_t u = -\lambda u + u^2, \quad u(0) = u_0, \quad t > 0.$$

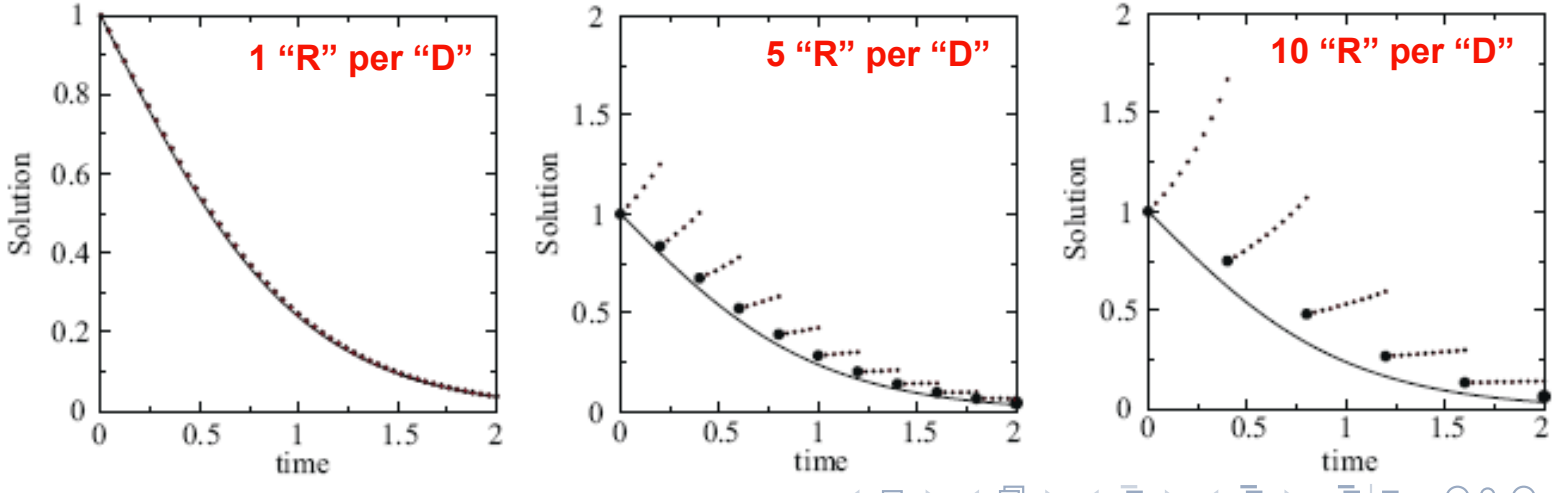
Phase 1 (R): $\partial_t u_r = u_r^2, \qquad u_r(t_n) = u_n, \qquad t \in [t_n, t_{n+1}]$,

Phase 2 (D): $\partial_t u_d = -\lambda u_d, \quad u_d(t_n) = u_r(t_{n+1}), \quad t \in [t_n, t_{n+1}]$.

True solution, $u(t) = \dfrac{u_0 e^{-\lambda t}}{1 + \frac{u_0}{\lambda}\left(e^{-\lambda t} - 1\right)}$, is well-defined $\forall t$ if $\lambda > u_0$.

Split solution, $u(t_{n+1}) = \dfrac{u(t_n) e^{-\lambda h}}{1 - u(t_n) h}$, can blow up in finite time.

Results using 50 time steps, with varying amounts of subcycling.



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Time Step Selection

Stability:
If IRK portion is A-stable, linear instability can only arise due to the ERK, so time steps must satisfy the explicit stability restriction,

$$h \leq h_{exp}.$$

Accuracy:
For an order q method with order p embedding (typically $q = p + 1$),

$$\begin{aligned} \|u(t_{n+1}) - u_{n+1}\| &\leq \|\tilde{u} - u_{n+1}\| + \|u(t_{n+1}) - \tilde{u}\| \\ &\leq \|\tilde{u} - u_{n+1}\| + \mathcal{O}(h^{p+1}). \end{aligned}$$

Hence h adaptivity may utilize $\|\tilde{u} - u_{n+1}\|$ for error estimation, e.g.

$$h_{n+1} = c\, h_n \left(\frac{r_{tol}}{\|\tilde{u} - u_{n+1}\|} \right)^{1/(p+1)}$$

In practice, a variety of adaptivity methods may be used, and are often based on control-theoretic techniques (e.g. I, PI, PID) [Gustafsson 1991 & 1994; Söderlind 2003].

Implicit Predictors and Dense Output

Accurate initial guesses are critical for nonlinear solver efficiency & robustness.

Each stage approximates the solution at a different time, i.e. $z_i \approx y(t_n + c_i h)$, giving rise to an interpolating polynomial (a.k.a. *dense output*),

$$u_d(t) = u_n + h \sum_{i=1}^{s} \left(\left(\sum_{j=1}^{p^*} b^*_{i,j} \left(\frac{t - t_n}{h} \right)^j \right) f(t_{n,i}, z_i) \right).$$

- Coefficients $b^*_{i,j}$ may be determined *a priori* for each method.
- $u_d(t)$ accuracy is limited by order of each z_i (typically lower than q).
- Extrapolation accuracy rapidly diminishes for $t > t_{n+1}$. Hence predictors are most helpful for early stages of next step.
- Later stages z_i may instead be predicted by previous stages, $z_1, \ldots z_{i-1}$.