Spectral deferred corrections with fast-wave slow-wave splitting

ECMWF Workshop on numerical and computational methods for simulation of all-scale geophysical flows

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Physically insignificant fast waves

https://www.youtube.com/watch?v=ieILUnkdD90

Image: NOAA

Figure: "Ten years of weather in 3 minutes".

- Acoustic waves have essentially no impact on larger scale atmospheric dynamics but severely restrict the time step:

  e.g. 2000 m grid resolution divided by $300\,\mathrm{m\,s^{-1}} \approx \Delta t \leq 6.7\,\mathrm{s}$

How to cope?

- Change the model: anelastic or pseudo-incompressible equations: remove acoustic waves from the system
- Use explicit integration with sub-stepping, e.g. RK-3 for advection and forward-backward Euler for acoustic terms
- Or: go IMEX. Integrate fast terms implicitly and slow terms explicitly.
  - Higher order methods can be difficult to derive, many order conditions!
  - Increasing order can reduce stability

...wouldn't it be nice to have an *easy* way to construct an IMEX integrator?

Collocation

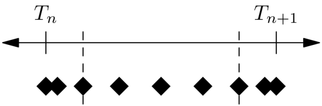


Figure: A time-step $[T_n, T_{n+1}]$ with $M = 9$ Gauss-Lobatto collocation nodes t_j.

- Consider Picard formulation of IVP

$$u(T_{n+1}) = u(T_n) + \int_{T_n}^{T_{n+1}} f(\tau, u(\tau))\, d\tau$$

- Approximation of integral by quadrature leads to collocation problem

$$\mathbf{U} = \mathbf{U}_0 + \Delta t \mathbf{QF}(\mathbf{U}), \ \mathbf{U} = (u_1, \dots, u_M)^{\mathrm{T}} \in \mathbb{R}^{NM \times NM}$$

with $u_j \approx u(t_j)$ approximations at the quadrature nodes

- Collocation methods are a subclass of implicit Runge Kutta methods[1]

[1] Hairer, Nørsett, and Wanner 1993, Theorem 7.7.

Spectral deferred corrections (SDC)[2]

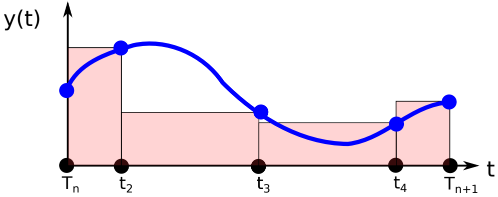


Figure: Composite rectangular rule $\mathbf{Q}_\Delta$ (red) as "preconditioner" for collocation rule $\mathbf{Q}$ (blue)

- SDC can be considered as a preconditioned Richardson iteration

$$\mathbf{U}^{k+1} = \mathbf{U}^k + (\mathbf{I} - \Delta t \mathbf{Q}_\Delta \mathbf{F})^{-1} \left[\mathbf{U}_0 - (\mathbf{I} - \Delta t \mathbf{Q} \mathbf{F}) \mathbf{U}^k \right], \quad \mathbf{Q}_\Delta \approx \mathbf{Q}, \quad \mathbf{U} \in \mathbb{R}^{NM}$$

  with $\mathbf{U}^k = (\mathbf{u}_1, \ldots, \mathbf{u}_M)^{\mathrm{t}}$.

- Or, in "node-to-node" form,

$$u_{m+1}^{k+1} = u_m^{k+1} + \Delta t_m f(u_{m+1}^{k+1}) - \Delta t_m f(u_{m+1}^k) + \sum_{j=1}^{M} s_{m,j} f(u_j^k)$$

  so that one iteration step $k \to k+1 \Leftrightarrow$ one "sweep" with implicit Euler

[2] Dutt, Greengard, and Rokhlin 2000, *BIT Numerical Mathematics*.

SDC with fast-wave slow-wave splitting

- For $f(y) = f_f(y) + f_s(y)$, instead of backward Euler

$$u_{m+1}^{k+1} = u_m^{k+1} + \Delta t_m f(u_{m+1}^{k+1}) - \Delta t_m f(u_{m+1}^k) + \sum_{j=1}^{M} s_{m,j} f(u_j^k),$$

can use IMEX as base method ("preconditioner") in SDC[3]

$$u_{m+1}^{k+1} = u_m^{k+1} + \Delta t_m \left[f_f(u_{m+1}^{k+1}) + f_s(u_m^{k+1}) + f_f(u_{m+1}^k) + f_s(u_m^k) \right] + \sum_{j=1}^{M} s_{m,j} f(u_j^k)$$

- In previous works, stiff/fast term from diffusion or chemical reaction[4]
- But: what about a fast *waves*, e.g. acoustic waves?
  → SDC with *fast-wave slow-wave splitting* ("fwsw-sdc")[5]

[3] Minion 2003, *Communications in Mathematical Sciences*.

[4] Layton and Minion 2004, *Journal of Computational Physics*.

[5] Ruprecht and Speck 2016, *SIAM Journal on Scientific Computing*.

Two views on convergence of SDC

Theorem: SDC as iterative solver

For $y' = f(y) = \lambda y$ and $|\lambda| \, \Delta t < 1$, the *error propagation matrix* $\mathbf{E}_{\mathrm{sdc}}$ of the SDC iteration satisfies

$$\left\| \mathbf{E}_{\mathrm{sdc}} \right\|_{\infty} \leq \frac{(1 + \Lambda_n) \, \Delta t \, |\lambda|}{1 - \Delta t \, |\lambda|} = \mathcal{O}(\Delta t) \text{ as } \Delta t \to 0$$

where Λ_n is the Lebesgue constant for the collocation nodes $(\tau_m)_{m=1,\dots,M}$.

Theorem: SDC to generate methods of fixed high order

The *local truncation error* of SDC based on a quadrature rule with order p with a fixed number of K iterations is

$$\left| u(T_{n+1}) - u_{n+1}^{K} \right| = \mathcal{O}(\Delta t^{\min\{K+1, p+1\}}) \text{ as } \Delta t \to 0.$$

Order of convergence

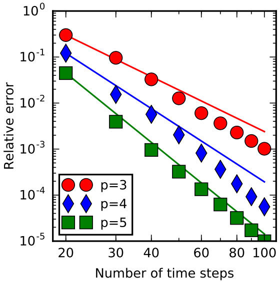


Figure: Convergence of SDC order $p=3$, $p=4$, $p=5$.

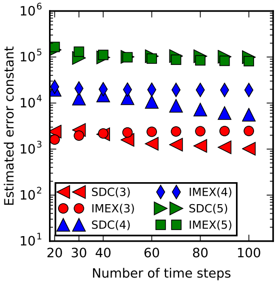


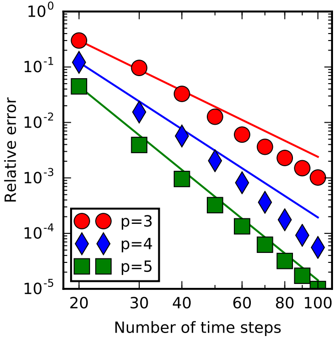
Figure: Estimated error constants of SDC and IMEX Runge-Kutta.

Acoustic-advection equations:

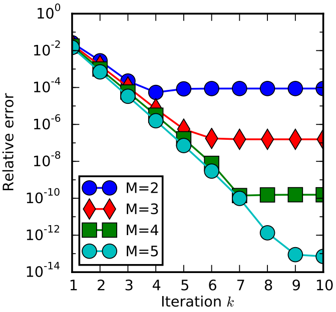
$$u_t + Uu_x + c_s p_x = 0$$
$$p_t + Up_x + c_s u_x = 0$$

with $u(x,0) = \sin(2\pi x) + \sin(10\pi x)$.

Two views on SDC



(a) Relative error versus time step Δt



(b) Relative error versus iteration k

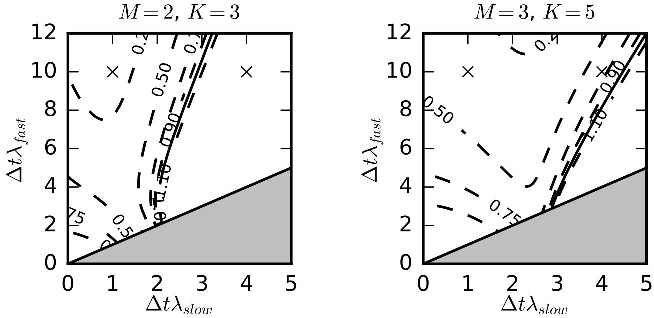
Figure: Convergence of SDC in Δt (left) and k (right) for $u'(t) = i\lambda_{fast} u(t) + i\lambda_{slow} u(t)$.

Can view SDC as...[1]

- framework to generate method of fixed order
- iterative solver for collocation problem

[1] Code available from `https://github.com/Parallel-in-Time/pySDC`

Stability of FWSW-SDC



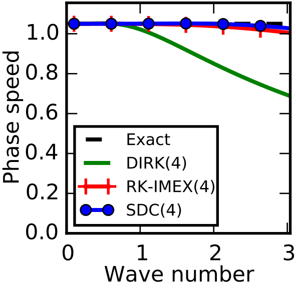
(a) Third-order (b) Fifth-order

- Stability of SDC with fast-wave slow-wave splitting for test problem

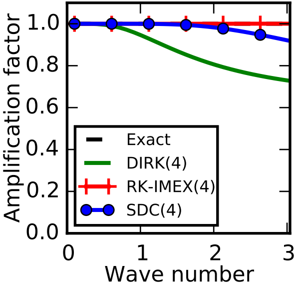
$$u'(t) = \underbrace{i\lambda_{\text{fast}} u(t)}_{\textit{implicit}} + \underbrace{i\lambda_{\text{slow}} u(t)}_{\textit{explicit}}, \quad u(0) = 1, \quad \lambda_{\text{fast}}, \lambda_{\text{slow}} \in \mathbb{R}.$$

- Choice of nodes critical to get stability for $\Delta t \lambda_{\text{fast}} \gg 1$.

Dispersion relation



(a) Phase speed Real(ω)/κ.



(b) Amplification factor exp (Imag(ω)).

Figure: Discrete dispersion relation for SDC, DIRK-RK and IMEX-RK.

- Connection between frequency ω and wave number κ in semi-discrete acoustic-advection problem

$$u_t + U u_x + c_s p_x = 0$$
$$p_t + U p_x + c_s u_x = 0$$

- Continuous dispersion relation $\omega = (U \pm c_s)\,\kappa$.

Multi-scale initial data[6]

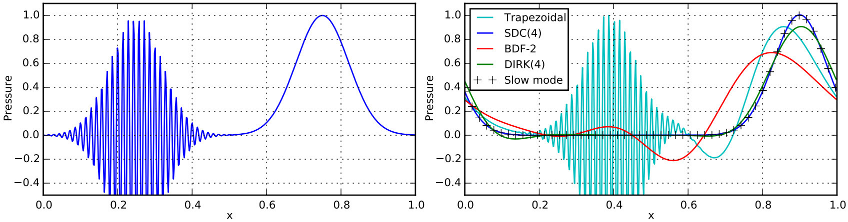


Figure: Multi-scale initial data (left). Pressure at $T = 3$ for four different methods (right).

Acoustic-advection equations:

$$u_t + U u_x + c_s p_x = 0$$
$$p_t + U p_x + c_s u_x = 0$$

with multi-scale initial data.

[6] Vater, Klein, and Knio 2011, *Acta Geophysica*.

Compressible two-dimensional linear Boussinesq equations

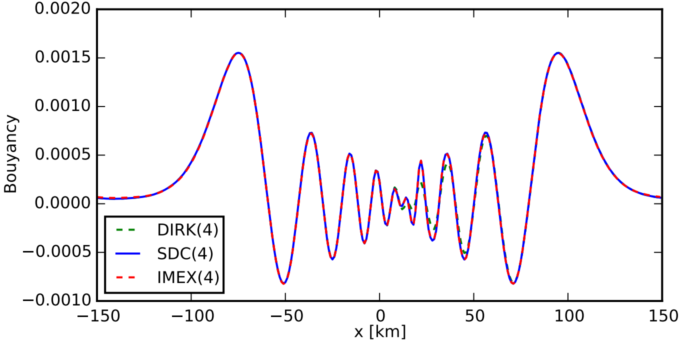


Figure: Gravity wave propagating in a channel.

Equations:

$$u_t + Uu_x + c_s p_x = 0$$
$$w_t + Uw_x + c_s p_z = b$$
$$b_t + Ub_x + N^2 w = 0$$
$$p_t + Up_x + c_s (u_x + w_z) = 0$$

- Count total number of GMRES iterations in implicit part
- IMEX-RK and FWSW-SDC solve red terms implicitly
- DIRK solves everything implicitly

GMRES iterations

Third-order	$\Delta t = 30\,$s			$\Delta t = 6\,$s		
	DIRK	IMEX	SDC	DIRK	IMEX	SDC
# implicit solves	200		900	1000	2000	4500
# GMRES iterations	46,702		25,819	28,863	13,782	25,051
avg. it. per call	233.5		28.7	28.9	6.9	5.6
est. error	1.8e-1	unstable	1.1e-1	9.6e-2	1.7e-2	1.5e-2

Fourth-order	$\Delta t = 30\,$s			$\Delta t = 6\,$s		
	DIRK	IMEX	SDC	DIRK	IMEX	SDC
# implicit solves	300	500	1200	1500	2500	6000
# GMRES iterations	100,651	38,092	31,105	66,136	24,068	32,696
avg. it. per call	335.5	76.2	25.9	44.1	9.6	5.4
est. error	1.5e-1	1.3e-1	9.9e-2	9.4e-2	4.2e-3	2.9e-3

Fifth-order	$\Delta t = 30\,$s			$\Delta t = 6\,$s		
	DIRK	IMEX	SDC	DIRK	IMEX	SDC
# implicit solves	500		1500	2500	3500	7500
# GMRES iterations	38,334		34,732	24,592	24,649	32,724
avg. it. per call	76.7		23.2	9.8	7.0	4.4
est. error	9.6e-2	unstable	9.7e-2	3.4e-3	2.7e-3	2.6e-3

FWSW-SDC – Summary

- Spectral deferred corrections are an easy way to generate high order time integration schemes
- Can use as framework with different integrators as base method: Boris, IMEX Euler, ...
- FWSW-SDC produces high order methods with fast-wave slow-wave splitting ... it has favourable properties and is less expensive than you might think!
- For more information please see Daniel Ruprecht and Robert Speck (2016). "Spectral Deferred Corrections with Fast-wave Slow-wave Splitting". In: *SIAM Journal on Scientific Computing* 38.4, A2535–A2557. DOI: 10.1137/16M1060078. URL: http://dx.doi.org/10.1137/16M1060078

The PinT Community

To learn more about parallel-in-time integration, check the new website

`www.parallelintime.org`

and/or come to one of the PinT Workshops, e.g.

5th Workshop on Parallel-in-Time Integration

- Nov 27 - Dec 2, 2016
- Banff International Research Station (BIRS), Calgary (CA)
- by M. Emmett, M. Gander, R. Haynes, R. Krause, M. Minion

There is also a new mailing list, join by writing to

`parallelintime+subscribe@googlegroups.com`

No Google account required!