TIME-PARALLEL IMEX TIME INTEGRATION BASED ON SPECTRAL DEFERRED CORRECTION

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Usual dilemma with time-integration

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Hamburg University of Technology

Choice between :

Explicit time integration

- simple to implement, but limited time-step size for numerical stability
- good old RK4 quite hard to beat $\rightarrow$ limited potential for improvement

$\Rightarrow$ usually more adapted to (non-linear) advection-dominated problems

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When you can't choose, simply take both : Implicit-Explicit methods (IMEX)

$$M\frac{\partial U}{\partial t} - L.U(t) = \mathcal{N}\left(U(t), t\right), \quad U(0) = U_0 \in \mathbb{C}^{N_{DoF}}$$

- L : linear operator (diffusive part), solved **implicitly**
- $\mathcal{N}$: non-linear operator (advective part), solved **explicitly**
- M : mass matrix, (singular) **such that** $M - \alpha L$ is invertible for any $\alpha \in]0, +\infty[$

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Most IMEX implementations require 3 main routines :

- `evalL(U)` : evaluate L on a solution U
- `evalN(U,t)` : evaluate $\mathcal{N}$ on a solution U at time t
- `linSolve(alpha,rhs)` : solve $(M - \alpha L)U = rhs$ for any rhs and α

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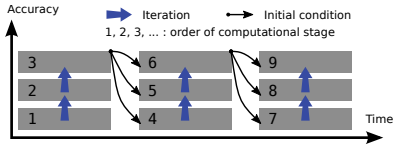
Spectral Deferred Correction : very good challenger to current state-of-the art for IMEX

Once upon a PinT ... Spectral Deferred Corrections



SDC[1] was introduced in 2000 on the basis of Deferred Correction[2]

[1] Dutt, Greengard, and Rokhlin, 2000. *"Spectral deferred correction methods for ordinary differential equations"*.

[2] Fox, 1947. *"Some improvements in the use of relaxation methods for the solution of ordinary and partial differential equations"*.

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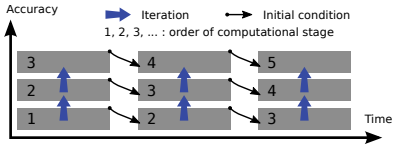

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$\Rightarrow$ induced many contributions to **parallel in time (PinT)** since then :

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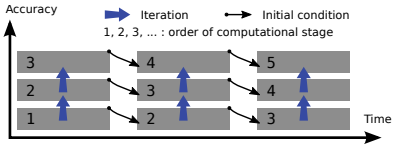

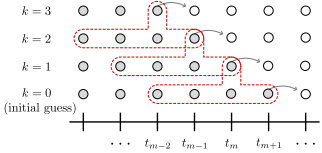

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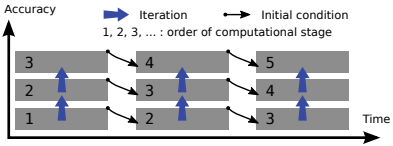

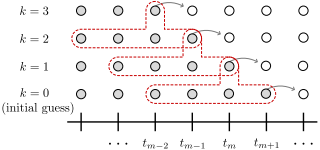

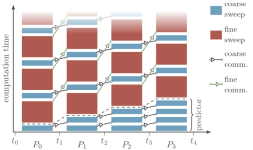

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- 2012 : multi-level sweeps with parallel fine sweep across the steps (PFASST)[5]

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1. consider the ODE system :

$$\frac{du}{dt} = f(u,t) \qquad t \in [0, \Delta t], \quad u(0) = u_0$$

2. write it into Picard form :

$$u(t) = u_0 + \int_0^t f(u(s), s)\, \mathrm{d}s, \qquad 0 \leq t \leq \Delta t$$

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3. use a given quadrature rule to approximate the integral on M **nodes** τ_m :

$$u_m = u_n + \Delta t \sum_{j=1}^{M} q_{m,j} f(u_j, \tau_j), \quad m = 1, \ldots, M, \quad \tau_m \in [0,1]$$

$$\Rightarrow \textbf{Collocation method}$$

Fully implicit M-stage Runge-Kutta methods

$$\begin{array}{c|ccc} \tau_1 & q_{1,1} & \dots & q_{1,M} \\ \vdots & \vdots & & \vdots \\ \tau_M & q_{1,M} & \dots & q_{M,M} \\ \hline & \omega_1 & \dots & \omega_M \end{array}$$

Node solutions computation can be seen as a **all-at-once system** :

$$\mathbf{u} - \Delta t Q f(\mathbf{u}) = \mathbf{u}_0, \quad \mathbf{u} = [.., u_m, ..], \quad \mathbf{u}_0 = [u_0, .., u_0]$$

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Once node solutions u_m (stages) are known, we perform (or not) the **step update** :

$$u_{n+1} = u_n + \Delta t \sum_{j=1}^{M} \omega_j f(u_j, \tau_j)$$

SDC $\Leftrightarrow$ *approximate the all-at-once with an* **iterative method** *(iterative Runge-Kutta)*

Solve iteratively the all-at-once system : $(I - \Delta t Q f)\mathbf{u} = \mathbf{u}_0$

4. consider the Picard iteration :

$$\mathbf{u}^{k+1} = \mathbf{u}^k + \left[\mathbf{u}_0 - (I - \Delta t Q f)\mathbf{u}^k\right]$$

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6. build P with a **lower triangular approximation** of Q :

$$Q_\Delta \simeq Q \quad \Rightarrow \quad P := (I - \Delta t Q_\Delta f) \quad \Rightarrow \text{direct solution with backward substitution}$$

$\rightarrow$ *repeat* K *times the SDC iteration, a.k.a* **sweep**

$$\mathbf{u}^{k+1} = \mathbf{u}^k + (I - \Delta t Q_\Delta f)^{-1} \left[\mathbf{u}_0 - (I - \Delta t Q f)\mathbf{u}^k \right]$$

Backward Euler based SDC (implicit) :

$$\mathbf{Q}_\Delta^{BE} = \begin{pmatrix} \Delta\tau_1 & & & \\ \Delta\tau_1 & \Delta\tau_2 & & \\ \vdots & & \ddots & \\ \Delta\tau_1 & \dots & \dots & \Delta\tau_M \end{pmatrix}$$

$$u_m^{k+1} = u_n + \Delta t \sum_{j=1}^{M} q_{m,j} f(u_j^k, \tau_j) + \Delta t \sum_{j=1}^{m} \Delta\tau_j [f(u_j^{k+1}, \tau_j) - f(u_j^k, \tau_j)]$$

- quadrature terms
- correction terms

$$\mathbf{u}^{k+1} = \mathbf{u}^k + (I - \Delta t Q_\Delta f)^{-1} \left[\mathbf{u}_0 - (I - \Delta t Q f)\mathbf{u}^k \right]$$

Forward Euler based SDC (explicit) :

$$\mathbf{Q}_\Delta^{FE} = \begin{pmatrix} 0 & & & \\ \Delta\tau_2 & 0 & & \\ \vdots & & \ddots & \\ \Delta\tau_2 & \dots & \Delta\tau_M & 0 \end{pmatrix}$$

$$u_m^{k+1} = u_n + \Delta t \sum_{j=1}^{M} q_{m,j} f(u_j^k, \tau_j) + \Delta t \sum_{j=1}^{m-1} \Delta\tau_{j+1} [f(u_j^{k+1}, \tau_j) - f(u_{j-1}^k, \tau_{j-1})]$$

- quadrature terms
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More expensive than classical methods (RK, Multistep, ...) **but** several advantages :

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4. high numerical stability with explicit forms
5. very high modularity (quadrature nodes, K, Q_Δ coefficients, ...)

$\Rightarrow$ very good **design framework** for the next generation time-integration methods

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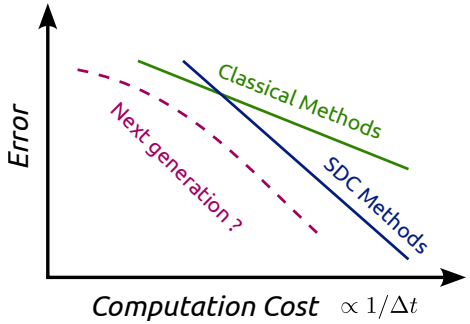
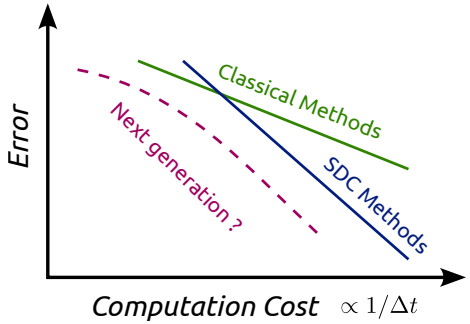
Better error *vs.* cost ratio

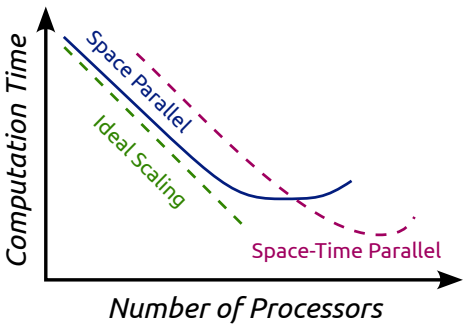


Main objectives

Better error *vs.* cost ratio



Better parallel efficiency



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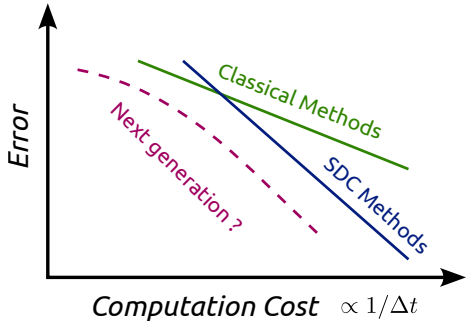

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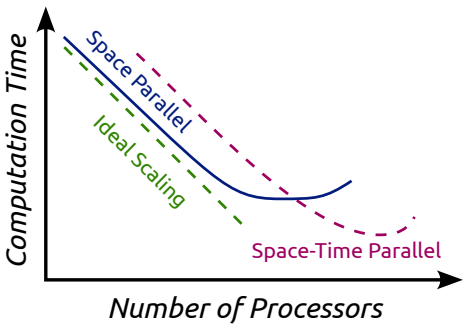

$\rightarrow$ *here is a first glitch of what can be done with SDC ...*

Parallel Diagonal SDC[7,8] : base idea

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Consider a diagonal $\mathbf{Q}_\Delta$ matrix :
$\Rightarrow$ time-parallel sweeps across nodes !

... *how to choose the coefficients* ?

$$\mathbf{Q}_\Delta^{diag} = \begin{pmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_M \end{pmatrix}$$

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... *how to choose the coefficients* ?
$\rightarrow$ write the SDC iteration matrix on Dahlquist problem :

$$\boldsymbol{e}^{k+1} = \mathbf{K}(\lambda\Delta t)\boldsymbol{e}^k \quad \Rightarrow \quad \mathbf{K}(\lambda\Delta t) = \lambda\Delta t(\mathbf{I} - \lambda\Delta t\mathbf{Q}_\Delta)^{-1}(\mathbf{Q} - \mathbf{Q}_\Delta)$$

$\rightarrow$ find the d_m coefficients minimizing the spectral radius of :

1. $\mathbf{I} - \mathbf{Q}_\Delta^{-1}\mathbf{Q} = \lim_{|\lambda\Delta t|\rightarrow\infty} \mathbf{K}(\lambda\Delta t)$ (stiff limit)
2. $\mathbf{Q} - \mathbf{Q}_\Delta = \lim_{|\lambda\Delta t|\rightarrow 0} \frac{\mathbf{K}(\lambda\Delta t)}{\lambda\Delta t}$ (non-stiff limit)

[7] Houwen and Sommeijer, 1991. *"Iterated Runge–Kutta methods on parallel computers"*.

[8] Speck, 2018. *"Parallelizing spectral deferred corrections across the method"*.

Parallel Diagonal SDC[9] : proposed solution

Look at **nilpotency** (and polynomials) rather than spectral radius (ill-conditioned)

[9] Čaklović et al., 2025. *"Improving Efficiency of Parallel Across the Method Spectral Deferred Corrections"*.

Look at **nilpotency** (and polynomials) rather than spectral radius (ill-conditioned)
$\Rightarrow$ three candidates :

1. `MIN-SR-NS` : $\mathbf{Q}_\Delta = diag(\tau_1/M, .., \tau_M/M)$ makes $\mathbf{Q} - \mathbf{Q}_\Delta$ nilpotent
2. `MIN-SR-S` : $\mathbf{Q}_\Delta$ that makes $\mathbf{I} - \mathbf{Q}_\Delta^{-1}\mathbf{Q}$ nilpotent, solving

$$\det((1-z)\mathbf{I} + z\mathbf{Q}_\Delta^{-1}\mathbf{Q}) = 1, \quad z \in \{\tau_1, ..., \tau_M\}$$

3. `MIN-SR-FLEX` : change $\mathbf{Q}_\Delta$ along iterations to make this matrix

$$(\mathbf{I} - \mathbf{Q}_\Delta^{-1}(M)\mathbf{Q}) \dots (\mathbf{I} - \mathbf{Q}_\Delta^{-1}(2)\mathbf{Q})(\mathbf{I} - \mathbf{Q}_\Delta^{-1}(1)\mathbf{Q})$$

nilpotent, using $\mathbf{Q}_\Delta(m) = diag(\tau_1/m, .., \tau_M/m)$

[9] Čaklović et al., 2025. *"Improving Efficiency of Parallel Across the Method Spectral Deferred Corrections"*.

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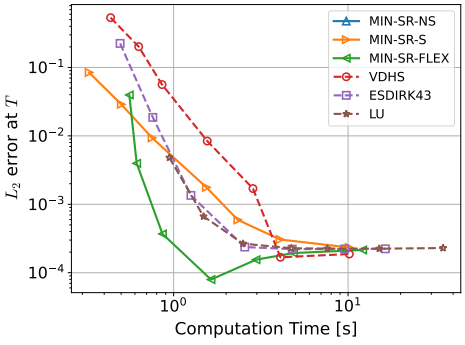
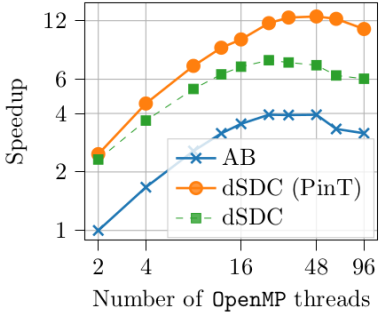
Implementation and evaluation of Parallel SDC sweeps :

1D non-linear Allen Cahn[a]



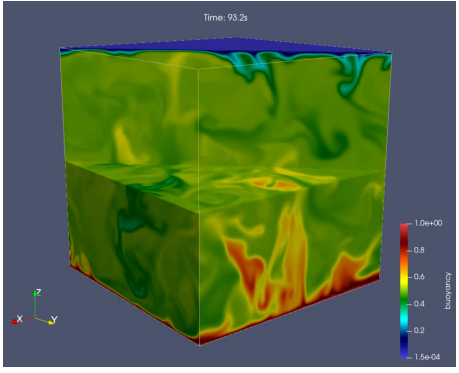
[a] Čaklović et al., 2025. *"Improving Efficiency of Parallel Across the Method Spectral Deferred Corrections"*.

2D shallow-water equations (sphere)[a]



[a] Freese et al., 2024. *"Parallel performance of shared memory parallel spectral deferred corrections"*.

Rayleigh-Bénard Convection in 3D



- turbulence induced by temperature gradient
- direct numerical simulation
- periodic boundary condition in x and y
- Dirichlet boundary condition in z
- velocities u_x, u_y, u_z, buoyancy b, pressure p

Depends on two dimensionless numbers :

1. Rayleigh Ra (turbulence)
2. Prandtl Pr (thermodynamic)

Normalized system of equations for the incompressible flow

$$\frac{\partial \mathbf{u}}{\partial t} - \sqrt{\frac{Pr}{Ra}}\Delta \mathbf{u} + \nabla p - b\mathbf{e}_z = \mathbf{u} \cdot \nabla \mathbf{u} \tag{1}$$

$$\frac{\partial b}{\partial t} - \frac{1}{\sqrt{RaPr}}\Delta b = \mathbf{u} \cdot \nabla b \tag{2}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{3}$$

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Pseudo-spectral space discretization (FFT-based) that solves the generic IMEX system :

$$M\frac{\partial U}{\partial t} - L.U(t) = \mathcal{N}\left(U(t), t\right), \quad U(0) = U_0 \in \mathbb{C}^{N_{DoF}}, \quad \text{with } M \text{ singular !}$$

$\Rightarrow$ *requires adapted time-integration schemes ...*

Time-integration using IMEX Runge-Kutta[10]

Stiffly accurate IMEX Butcher tables A and $\hat{A}$ with common stages $\mathbf{c}$

$$\begin{array}{c|cccc} 0 & 0 & 0 & \dots & 0 \\ c_1 & 0 & a_{1,1} & \dots & 0 \\ c_2 & 0 & a_{2,1} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & a_{M,1} & \dots & a_{M,M} \\ \hline & 0 & a_{M,1} & \dots & a_{M,M} \end{array} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & \dots & 0 \\ c_1 & \hat{a}_{2,1} & 0 & \dots & 0 \\ c_2 & \hat{a}_{3,1} & \hat{a}_{3,2} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \hat{a}_{s,1} & \hat{a}_{s,2} & \dots & 0 \\ \hline & \hat{a}_{s,1} & \hat{a}_{s,2} & \dots & 0 \end{array}$$

Time-stepping solves the **all-at-once system** to get $U_S = [U_1, \dots, U_s]^T$:

$$[I \otimes M - A \otimes L]\, U_S - \hat{A} \otimes \mathcal{F}(U_S, \mathbf{c}) = \mathbb{1} \otimes U_0$$

[10] Ascher, Ruuth, and Spiteri, 1997. *"Implicit-explicit Runge-Kutta methods for time-dependent partial differential equations"*.

Time-integration using IMEX Runge-Kutta[10]

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Stiffly accurate IMEX Butcher tables A and $\hat{A}$ with common stages $\mathbf{c}$

$$\begin{array}{c|cccc} 0 & 0 & 0 & \dots & 0 \\ c_1 & 0 & a_{1,1} & \dots & 0 \\ c_2 & 0 & a_{2,1} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & a_{M,1} & \dots & a_{M,M} \\ \hline & 0 & a_{M,1} & \dots & a_{M,M} \end{array} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & \dots & 0 \\ c_1 & \hat{a}_{2,1} & 0 & \dots & 0 \\ c_2 & \hat{a}_{3,1} & \hat{a}_{3,2} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \hat{a}_{s,1} & \hat{a}_{s,2} & \dots & 0 \\ \hline & \hat{a}_{s,1} & \hat{a}_{s,2} & \dots & 0 \end{array}$$

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$\Rightarrow$ stage-by-stage with backward substitution + **last stage as next step solution**

[10] Ascher, Ruuth, and Spiteri, 1997. *"Implicit-explicit Runge-Kutta methods for time-dependent partial differential equations"*.

Collocation matrix Q on the nodes τ (stages) to build the all-at-once problem :

$$\begin{array}{c|ccc} \tau_1 & q_{1,1} & \cdots & q_{1,s} \\ \vdots & \vdots & & \vdots \\ 1 & q_{1,s} & \cdots & q_{s,s} \\ \hline & q_{1,s} & \cdots & q_{s,s} \end{array}$$

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Use K IMEX sweeps on $U_S^k = [U_1^k, \dots, U_s^k]^T$ (solved with backward substitution)

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Use a diagonal "approximation" $Q_\Delta \Rightarrow$ **parallel IMEX sweeps across the stages**

Comparison with state of the art

Considering the same number of stages $s = 4$, $K = 4$ for SDC and some $\mathbf{Q}_\Delta$ ...

Runge-Kutta (RK443)

- third order accuracy
- maximum CFL at 1.57
- computational cost $\simeq N_{stages}$
- sequential stage computation

PIMEX SDC

- fourth order accuracy
- maximum CFL at 2.83
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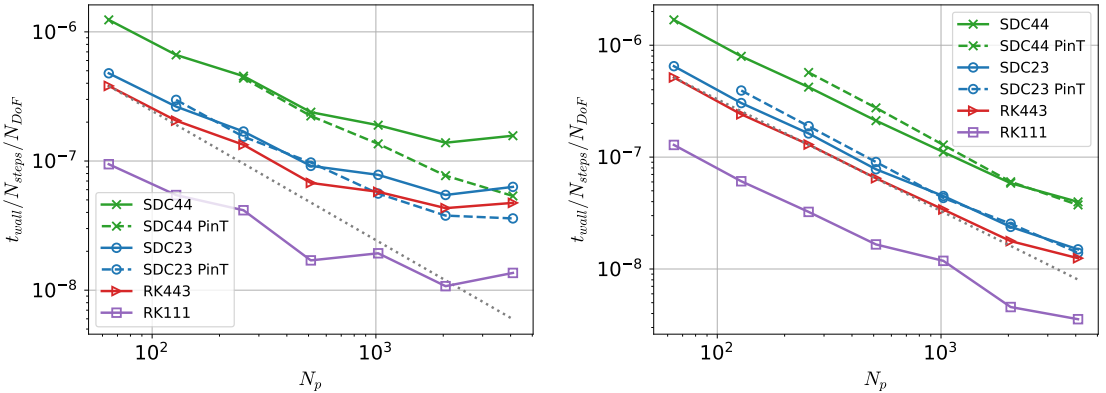
Faster time-to-solution for SDC with parallel-in-time (PinT) **and** *time-step increase ?*

Strong scaling tests for single time-step

RBC on a 32×128^2 (left) and 64×256^2 (right) grid, 50% CPU node load (Jusuf, JSC)



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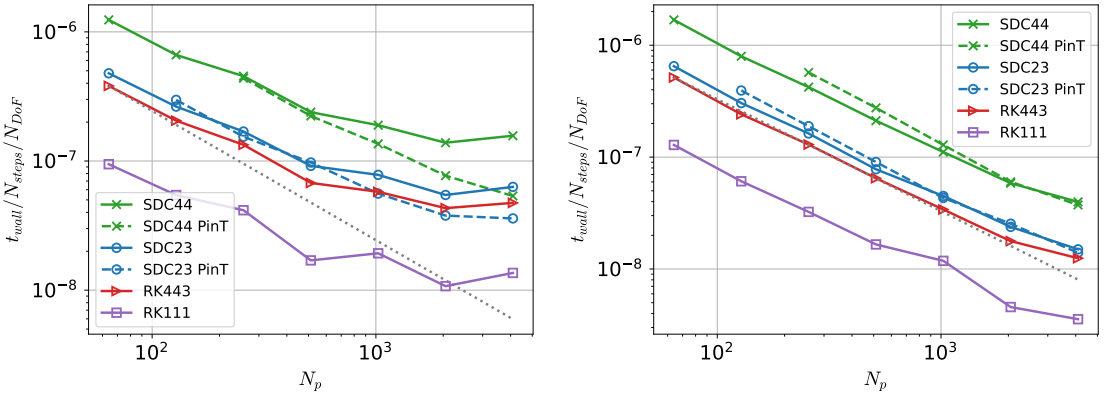

$\Rightarrow$ PIMEX SDC may win by a small margin, but **time-step size increase is crucial**

Numerical stability depending on Rayleigh number

Maximum time-step size and multiplicative factor vs RK111 :

Method	$Ra = 10^5$ $(128^2 \times 32)$	$Ra = 10^6$ $(256^2 \times 64)$	$Ra = 10^7$ $(512^2 \times 128)$
RK111	0.0526	0.00568	0.00144
RK443	0.0714 ($\times$1.4)	0.0147 ($\times$2.6)	0.0050 ($\times$3.5)
PIMEX SDC23	0.1000 ($\times$1.9)	0.0167 ($\times$2.9)	0.0056 ($\times$3.9)
PIMEX SDC44	0.0833 ($\times$1.6)	0.0192 ($\times$3.4)	0.0071 ($\times$4.9)

- stability advantages of PIMEX SDC increases with Ra
- projected computation time reduction using PinT around -20% for high Ra

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- projected computation time reduction using PinT around -20% for high *Ra*

... now we just need access to a larger HPC cluster to demonstrate that

In the meantime :
can this stability improvement be demonstrated (or improved) with analysis ?

Dahlquist problem : $\frac{du}{dt} = (z_I + z_E)u$, $\Delta t = 1$, stage solution vector $\mathbf{u} = [u_1, ..., u_s]^T$

- IMEX RK step (or general collocation) :

$$\left(\mathbf{I} - z_I A - z_E \hat{A}\right)\mathbf{u} = \mathbf{u}_0 \qquad (\mathbf{I} - (z_I - z_E)\mathbf{Q})\,\mathbf{u} = \mathbf{u}_0$$

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$$(\mathbf{I} - z_I \mathbf{Q}_\Delta)\,\mathbf{u}^{k+1} = \mathbf{u}_0 + (z_I + z_E)Q\mathbf{u}^k - z_I \mathbf{Q}_\Delta \mathbf{u}^k$$

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- generic IMEX SDC sweep :

$$\left(\mathbf{I} - z_I \mathbf{Q}_\Delta^I - z_E \mathbf{Q}_\Delta^E\right) \mathbf{u}^{k+1} = \mathbf{u}_0 + (z_I + z_E) Q \mathbf{u}^k - z_I \mathbf{Q}_\Delta \mathbf{u}^k - z_E \mathbf{Q}_\Delta^E \mathbf{u}^k$$

PIMEX SDC $\Leftrightarrow$ Picard for explicit ($\mathbf{Q}_\Delta^E = 0$), diagonal $\mathbf{Q}_\Delta$ coefficients for implicit

Advection-diffusion splitting

$$\frac{du}{dt} = (\lambda_I + i\lambda_E)u, \quad u_0 = 1, \quad \sqrt{i} = -1, \quad \lambda_I \in]-\infty, 0], \quad \lambda_E \in [0, +\infty]$$

$\rightarrow$ compute the numerical solution u_1 after one time-step $\Delta t = 1$, and look at :

1. amplification factor $|u_1|$: larger than 1 $\Rightarrow$ numerical instability
2. accuracy $|u_1 - e^{\lambda_I + i\lambda_E}|$: how accurate are we on each eigenvalue

[11] Ascher, Ruuth, and Spiteri, 1997. *"Implicit-explicit Runge-Kutta methods for time-dependent partial differential equations"*.

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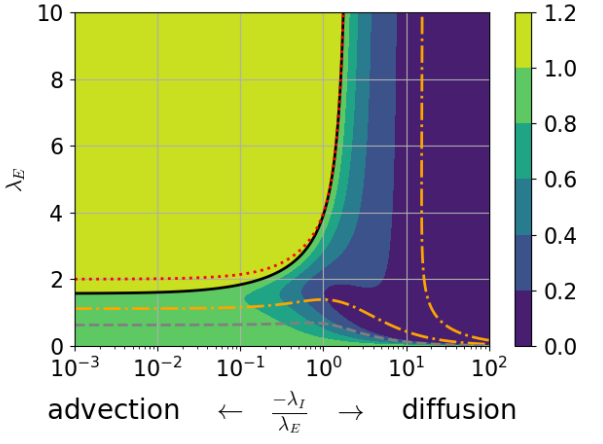
$\rightarrow$ contour plot[11] of those quantities in the $(-\lambda_I/\lambda_E, \lambda_E)$ plane ...

[11] Ascher, Ruuth, and Spiteri, 1997. *"Implicit-explicit Runge-Kutta methods for time-dependent partial differential equations"*.

Maximum CFL for $-\lambda_I/\lambda_E \to 0$
$\Rightarrow$ $CFL_{max} = 1.57$

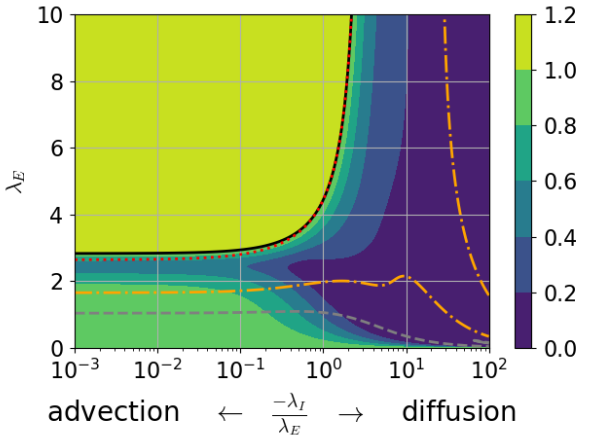
Accuracy contours

- gray dashes : 0.01
- orange dots-dashes : 0.1
- red dots : 1



PIMEX SDC44

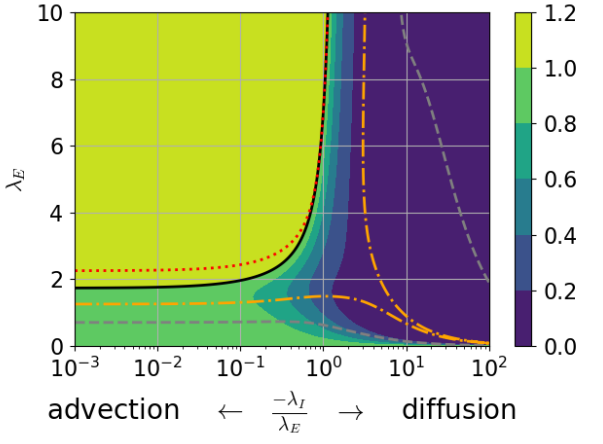
Maximum CFL for $-\lambda_I/\lambda_E \to 0$
$\Rightarrow$ $CFL_{max} = 2.83$ ($\times$ 1.8 vs RK443)



PIMEX SDC stability

PIMEX SDC23

Maximum CFL for $-\lambda_I/\lambda_E \to 0$
$\Rightarrow$ $CFL_{max} = 1.73$ ($\times$ 1.1 vs RK443)



Current limitations of this analysis

We don't really look at the effective values for λ_E and λ_I/λ_E ... we would also need :

- linearization of the governing equations for one time-steps
- expression depending on effective CFL and Ra
- taking into account 3D

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- expression depending on effective CFL and *Ra*
- taking into account 3D

But enough to get stability estimation and investigate other SDC variants ...

Idea : modify the implicit operator in SDC to increase stability[12] ... *because we can !*

$$\left(\mathbf{I} - (z_I - \frac{\theta}{2} z_E^2)\mathbf{Q}_\Delta\right)\mathbf{u}^{k+1} = \mathbf{u}_0 + (z_I + z_E)Q\mathbf{u}^k - (z_I - \frac{\theta}{2} z_E^2)\mathbf{Q}_\Delta \mathbf{u}^k$$

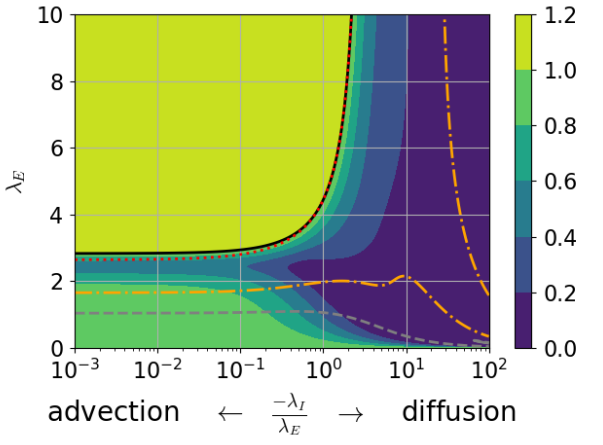
- used one major advantage of SDC : you can put **anything** in the preconditionner
- corresponds to subtracting a part of the advective term into the diffusive term
- loose a bit on accuracy, but gain a lot on numerical stability

[12] Stiller, 2025. *"Stable semi-implicit SDC methods for conservation laws"*.

Stabilized PIMEX SDC stability

SPIMEX SDC44, $\theta = 0.0$

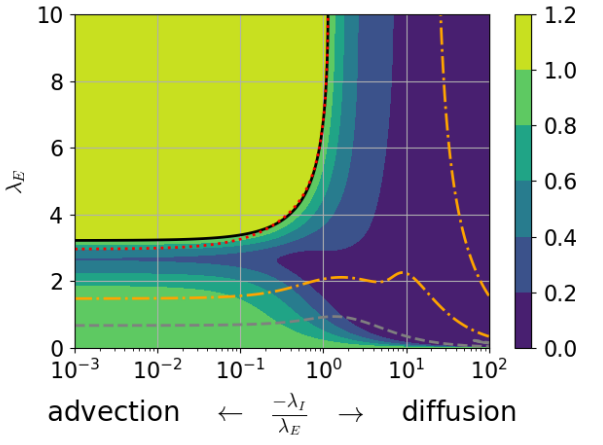
Maximum CFL for $-\lambda_I/\lambda_E \to 0$
$\Rightarrow$ $CFL_{max} = 2.83$ ($\times$ 1.8 vs RK443)



Stabilized PIMEX SDC stability

SPIMEX SDC44, $\theta = 0.1$

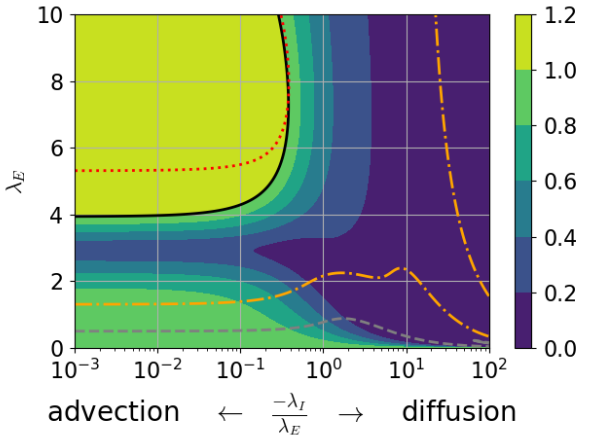
Maximum CFL for $-\lambda_I/\lambda_E \to 0$
$\Rightarrow$ $CFL_{max} = 3.22$ ($\times$ 2.1 vs RK443)



Stabilized PIMEX SDC stability

SPIMEX SDC44, $\theta = 0.2$

Maximum CFL for $-\lambda_I/\lambda_E \to 0$
$\Rightarrow$ $CFL_{max} = 3.94$ ($\times$ 2.5 vs RK443)



But why stop there ... we still can

- optimize diagonal coefficients for IMEX
- combine with multi-level or PFASST based approaches (second PinT layer)
- try other crazy ideas ...

Pandora's box still not fully opened yet !

Conclusions

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SDC is a generic framework to solve ODEs, with

1. high design flexibility and combination potential (multi-level / multi-scale, ...)
2. higher cost for better accuracy and numerical stability
3. natural direct time-parallelism with problem-independent speedup

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But finding a new rare gem requires :

- more people knowing how it works, with some time to spend on it
- proper analysis to determine optimal SDC coefficients for different cases
- efficient generic implementations to show off on large scale non-linear problems

$\Rightarrow$ we need developments in Applied Mathematics & HPC & RSE

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as Gear / Butcher said : lot more to do ...

SDC Days 2026 : gather people who are interested in SDC-based methods, or related time-integration in general ...

- 2022 : Hamburg (TUHH)
- 2023 : Jülich Supercomputing Center
- 2024 : Grenoble (INRIA)
- 2025 : Dresden (TUD)

$\Rightarrow$ next one around **16th December 2026 at TUHH**

more details to come ...