

PyPinT

Towards a framework for rapid prototyping of iterative parallel-in-time algorithms

May 28, 2014 | Torbjörn Klatt, Dieter Moser, Robert Speck | 3rd Workshop on Parallel-in-Time Integration

Overview

1 Recap of existing Parallel-in-Time Approaches

Parareal, (I)DC, (ML)SDC, PFASST

2 The *PyPinT* Framework Explained

concepts, design decisions, modules

3 Goals of *PyPinT*

creating a unicorn

4 Proof of Concept

coloured plots and pictures, yeah!



PyPinT

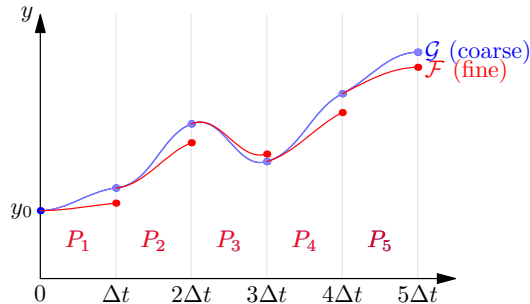
Part I: Existing Parallel-in-Time Approaches

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Parareal

Y. Maday. 2008. *The Parareal in Time Algorithm*.

- coarse \mathcal{G} and fine \mathcal{F} propagators make parareal flexible and modular
- an initial value is improved iteratively
- order is controllable through the fine propagator \mathcal{F}



[Courtesy of M. Emmett, LBNL]

$$y_{m+1}^{k+1} = \mathcal{F}(y_m^k) + \mathcal{G}(y_m^{k+1}) - \mathcal{G}(y_m^k)$$

What is needed? Two Integrators

Deferred Corrections

V. Pereyra. 1966. *On Improving an Approximate Solution of a Functional Equation by Deferred Corrections*. Numerische Mathematik. 8(4) 376–391.

$$y'(t) = f(t, y(t)), \quad y(0) = y_0$$

Using the residual

$$r(t) = f(t, \tilde{y}(t)) - \tilde{y}'(t)$$

to compute the error

$$e'(t) = f(t, \tilde{y} + e) - f(t, \tilde{y}) + r'(t)$$

$$e(0) = 0$$

for the next update

$$\tilde{y}_{j+1} = \tilde{y}_j + e_j$$

Deferred Corrections and Integral Deferred Corrections

A. Dutt, L. Greengard, V. Rokhlin. 2000. *Spectral Deferred Correction Methods for Ordinary Differential Equations*. BIT Numerical Mathematics 40(2) 241–266.

$$y'(t) = f(t, y(t)), \quad y(0) = y_0$$

$$y(t) = y_0 + \int_0^t f(\tau, y(\tau)) d\tau, \quad y(0) = y_0$$

Using the residual

$$r(t) = f(t, \tilde{y}(t)) - \tilde{y}'(t)$$

to compute the error

$$\begin{aligned} e'(t) &= f(t, \tilde{y} + e) - f(t, \tilde{y}) + r'(t) \\ e(0) &= 0 \end{aligned}$$

for the next update

$$\tilde{y}_{j+1} = \tilde{y}_j + e_j$$

Using the residual

$$r(t) = y_0 - \tilde{y}(t) + \int_0^t f(\tau, y(\tau)) d\tau$$

to compute the error

$$e(t) = \int_0^t f(\tau, \tilde{y} + e) - f(\tau, \tilde{y}) d\tau + r(t)$$

for the next update

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Spectral Deferred Corrections

A. Dutt, L. Greengard, V. Rokhlin. 2000. *Spectral Deferred Correction Methods for Ordinary Differential Equations*. BIT Numerical Mathematics 40(2) 241–266.



One sweep is performed by

$$u_{n+1}^{k+1} = u_n^{k+1} + \Delta t \left[F(u_{n+1}^{k+1}) - F(u_{n+1}^k) \right] + \mathcal{I}_n^{n+1} \left(F(u^k) \right)$$

new main constituent is the quadrature operator

$$\mathcal{I}_n^{n+1} \mathbf{y} = \sum_{i=1}^m \omega_i \tilde{y}_i \approx \int_{t_n}^{t_{n+1}} y(\tau) d\tau$$

What is needed? Quadrature, Evaluation of F (, Space Solver) \longrightarrow new Integrator

Multilevel SDC

R. Speck, D. Ruprecht, M. Emmett, M. L. Minion, M. Bolten, R. Krause. 2013. *A Multi-Level Spectral Deferred Correction Method*. arXiv Math Numerical Analysis.

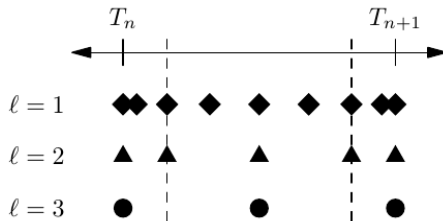
Slightly different sweep

$$u_{n+1}^{k+1} = u_n^{k+1} + \Delta t \left[F \left(u_{n+1}^{k+1} \right) - F \left(u_{n+1}^k \right) \right] + \mathcal{I}_n^{n+1} \left(F \left(u^k \right) \right) + \tau_n^k$$

and multiple level, correction τ_n^k based on information from different levels

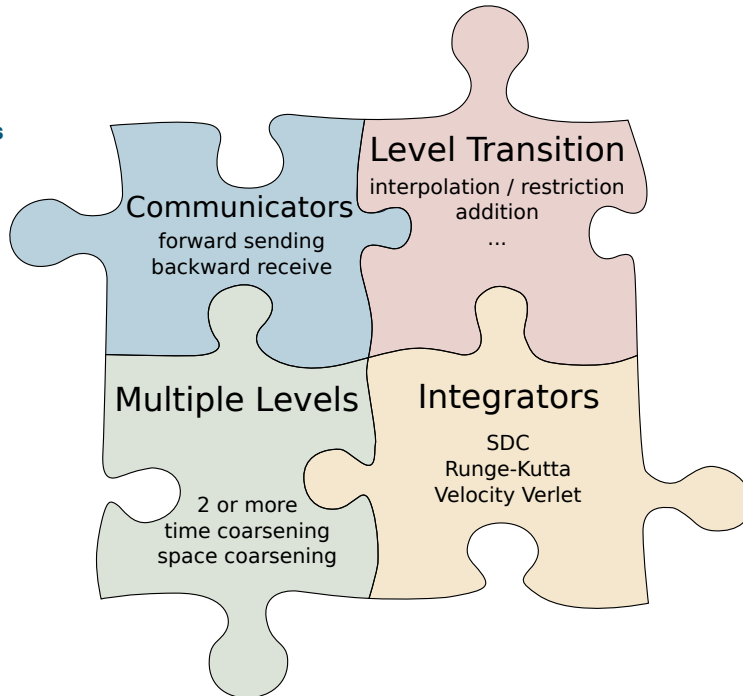
What is needed?

- same as SDC
- **Interpolation** (space and time)
- **Restriction** (space and time)



PFASST

Building Blocks





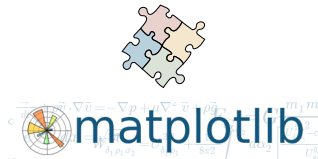
PyPinT

Part II: The PyPinT Framework Explained

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Basic Concept

- *Python* ≥ 3.2 as language of choice
for ease of use and extensibility (cf. *NumPy*, *SciPy*)
- modular building blocks
for fast exchange of algorithms' building blocks
- well-conceived and intuitive abstract interfaces
for reusable code ensuring DRY principle
- integrated analyzation tools
for introspection and plotting (cf. *matplotlib*)
- usage of a sophisticated unit-testing framework
nobody writes bug-free code

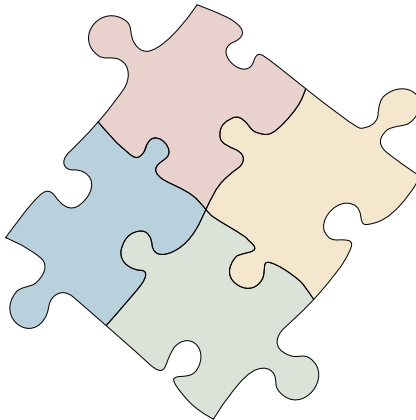


Modules

Abstract Modelling of PinT Algorithms

`pypint`

- `~.problems`
- `~.solvers`
- `~.integrators`
- `~.communicators`
- `~.multi_level_providers`
- `~.solutions`
- `~.plugins`



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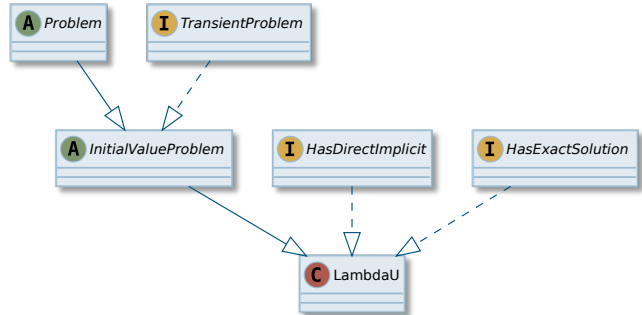
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- interfaces for problem setups
- generic problem with specializations via mixins



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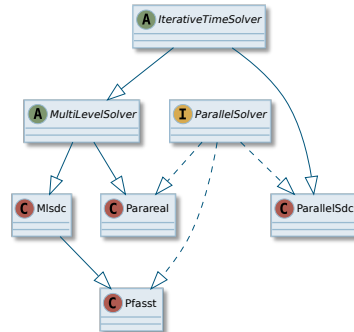
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- interfaces for iterative time solvers
- providing generic building blocks of solvers



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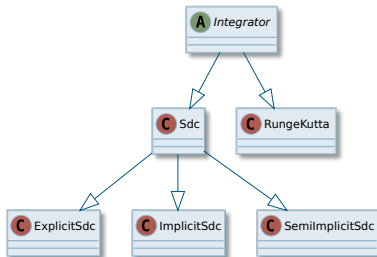
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- abstract interface for integrators of ODEs
e.g. *Runge-Kutta*, *Expl./Impl. Euler*, *SDC* etc.
- unified generic interface for executing integrator
via method `.apply(*args, **kwargs)`



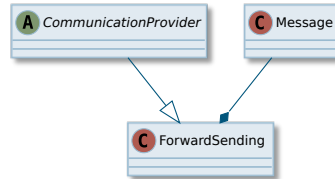
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```

- generic abstract interfaces for communication patterns
e.g. implemented as *forward sending*, etc.
- extendable basic message buffer
holding data, solver flags and other meta information



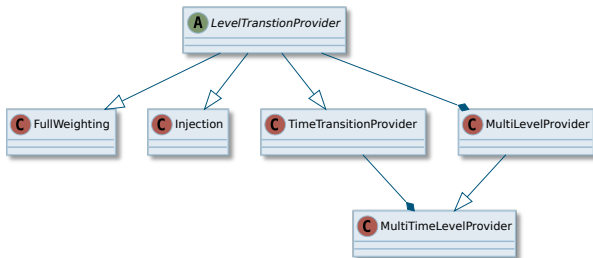
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```

- abstract interface for generic level transitions
e.g. *full weighting*, *injection*, *Lagrange-polynomial integration* etc.
- containers for multiple levels
providing access to integrators of each level
- unified generic interface for transitions between levels
via methods `.restrict(data, fine_id, coarse_id)` and `.prolongate(data, coarse_id, fine_id)`



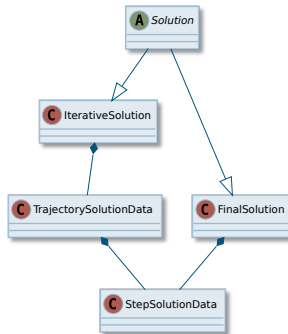
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- containers for solution data + meta information
e.g. time-node/step-wise, trajectory (consecutive time nodes)
- container interface for complete solutions
e.g. only last time node of last iteration or all nodes of all iterations



Modules

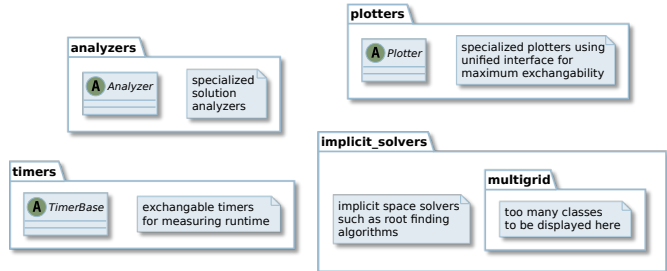
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PyPinT

Part III: Goals for PyPinT

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- open-source hosted on  GitHub
⇒ reaching young & rising developers and scientists promoting PinT algorithms



PyPinT

Part IV: Proof of Concept

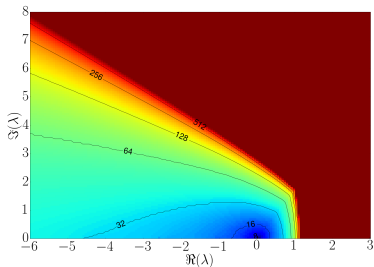
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Implementation of SDC and MLSDC

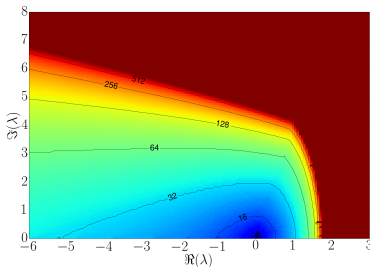
Convergence Regions (number iterations for residual $\leq 10^{-14}$) of $u'(x, t) = \lambda u(x, t)$, $t \in [0, 1]$, $\lambda \in \mathbb{C}$

SDC

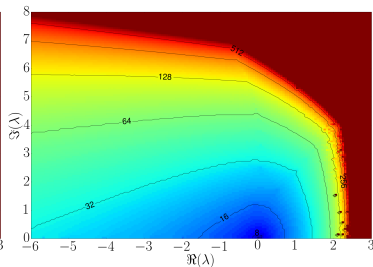
3 Gauss-Lobatto nodes



5 Gauss-Lobatto nodes



7 Gauss-Lobatto nodes



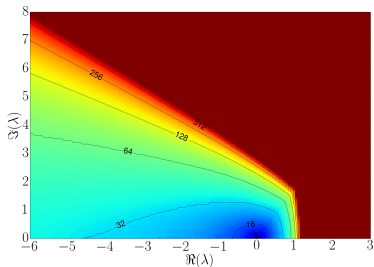
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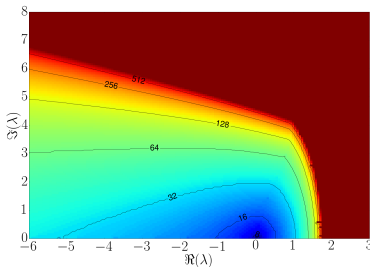
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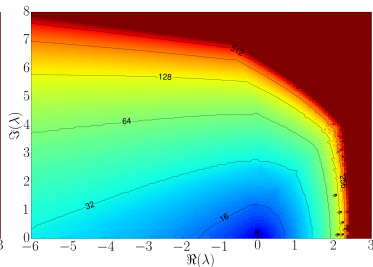
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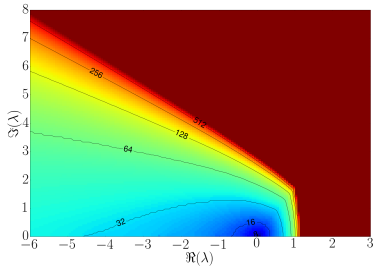


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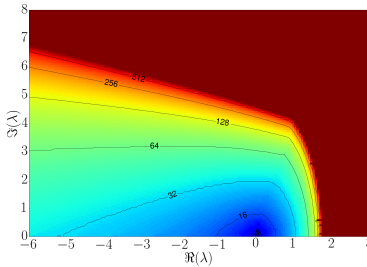
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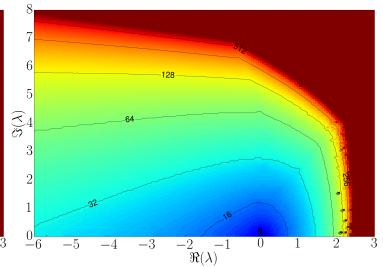
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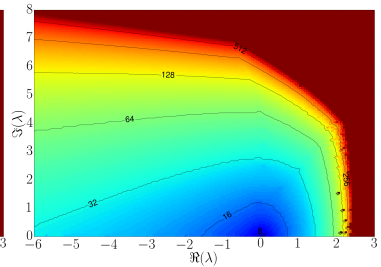
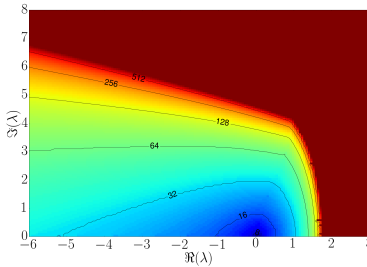
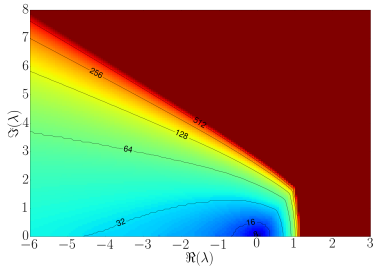
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SDC

3 Gauss-Lobatto nodes

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MLSDC



Implementation of SDC and MLSDC

Python Script for a SDC run with 3 Gauss-Lobatto nodes

```
1 prob = LambdaU(complex(-1.0, 1.0))
2 comm = ForwardSendingMessaging()
3 solver = Sdc(communicator=comm)
4 solver.init(problem=prob)
5 quadr = QuadratureBase(nodes=GaussLobatto(num_nodes=3),
6                               weights=Polynomial(coeffs=[1]))
7 integr = SemiImplicitSdc(quadrature=quadr)
8 solution = solver.run(integrator=integr)
9 # plotting via matplotlib.pyplot
```

The Aviles-Giga Problem

An example from *real* life ...

$$u_t = \frac{1}{\varepsilon} \underbrace{\nabla \cdot \left((|\nabla u|^2 - 1) \nabla u \right)}_{\mathcal{N}} - \varepsilon \nabla^4 u$$

The Aviles-Giga Problem

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- highly nonlinear part \mathcal{N}
- computed on a periodic domain $\mathbb{T} = (0, 2\pi)^2$

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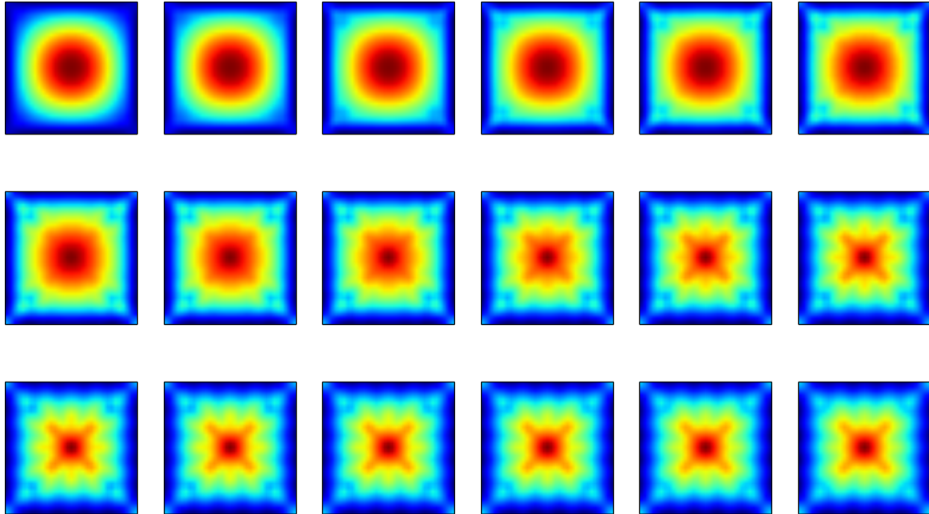
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But what is it good for?

It is a simple model for Pattern Forming Mechanisms in magnetic bulk

The Aviles-Giga Problem

... for nice plots ...



The Aviles-Giga Problem

...with less code

```
def evaluate_wrt_time(self, time, phi_of_time, **kwargs):
    """Computing the right hand side with respect to time
    """
    super(AvilesGiga, self).evaluate_wrt_time(time, phi_of_time, **kwargs)
    self._u.reshape(phi_of_time.shape[:]) = phi_of_time
    self._u_f = self.fft(self._u)
    self.compute_grad()
    if kwargs.get('partial') is not None:
        if isinstance(kwargs['partial'], str) and kwargs['partial'] == 'impl':
            return (- self.epsilon * self.compute_linear()).reshape(phi_of_time.shape)
        elif kwargs['partial'] == 'expl':
            return (self.compute_non_linear() / self.epsilon).reshape(phi_of_time.shape)
    else:
        return \
            (self.compute_non_linear() / self.epsilon - self.epsilon * self.compute_linear())\
            .reshape(phi_of_time.shape)

def implicit_solve(self, next_x, func, method="unused", **kwargs):
    """A solver for the implicit equations.
    """
    sol = scop.newton_krylov(func, next_x.reshape(-1))
    return sol.reshape(self.dim_for_time_solver)
```


Advantages of *PyPinT*

“towards” ...

- playground for rapid prototyping of PinT algorithms
 - no need to implement e.g. matrix inversion or quadrature on your own
⇒ saves your precious time
- use of Python's full feature set
 - easy parallelism
via Python's own (e.g. multiprocessing) or 3rd-party modules (e.g. mpi4py)
 - built-in portability
runs on Unix and MacOS (should run on Windows too)
 - interactive computing
integrates well with IPython


IP[y]: IPython
Interactive Computing



Thank you for your attention!

Questions?

(now or later)

PyPinT is on  GitHub: <https://github.com/Parallel-in-Time/PyPinT>

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