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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

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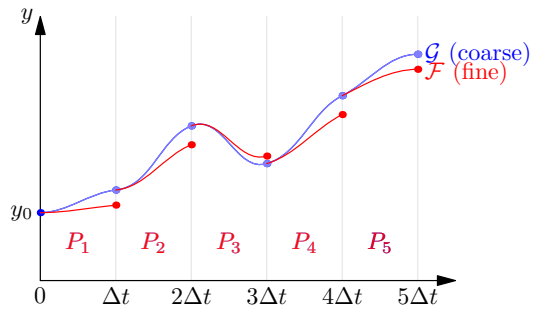
Part I: Existing Parallel-in-Time Approaches

May 28, 2014 | Torbjörn Klatt, Dieter Moser, Robert Speck

Parareal

Y. Maday, *The parareal in time algorithm*, pp. 1–24, 2008.

- 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, “On improving an approximate solution of a functional equation by deferred corrections,” Numer. Math., vol. 391, no. 044, pp. 376–391, 1966.

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

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, and V. Rokhlin, "Spectral deferred correction methods for ordinary differential equations," BIT Numer. Math., vol. 40, no. 2, pp. 241–266, Jun. 2000.

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for the next update

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

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

Using the residual

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

to compute the error

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

for the next update

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

Spectral Deferred Corrections

A. Dutt, L. Greengard, and V. Rokhlin, “Spectral deferred correction methods for ordinary differential equations,” BIT Numer. Math., vol. 40, no. 2, pp. 241–266, Jun. 2000.

One sweep is performed by

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

new main constituent is the quadrature operator

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

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

Multilevel SDC

R. Speck, D. Ruprecht, and M. Emmett, “A multi-level spectral deferred correction method,” arXiv Prepr. arXiv . . . , 2013.

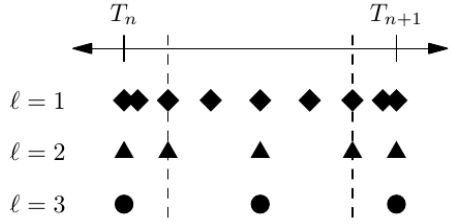
Slightly different sweep

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

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

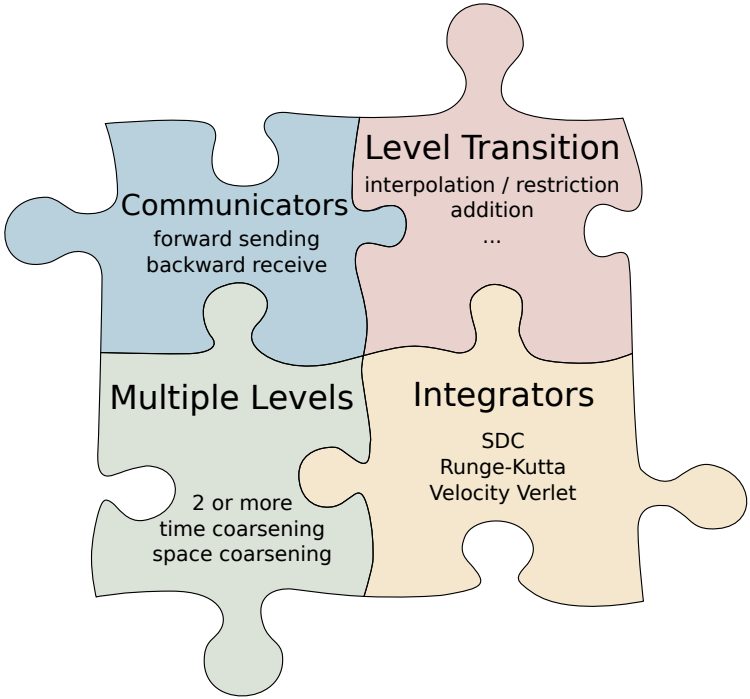
What is needed?

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



PFASST

Building Blocks



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Part II: The PyPinT Framework Explained

May 28, 2014 | Torbjörn Klatt, Dieter Moser, Robert Speck

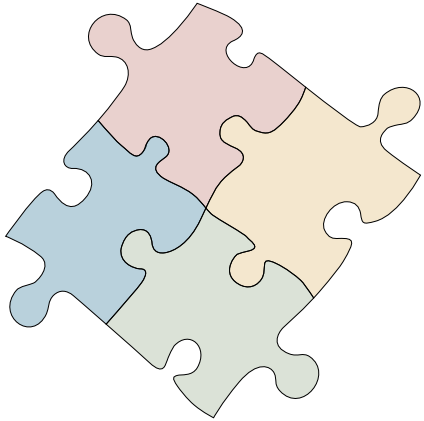
Basic Concept

- *Python* $\geq$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
  ~.integratos
  ~.communicators
  ~.multi_level_providers
  ~.quadrature
  ~.solutions
  ~.plugins
```



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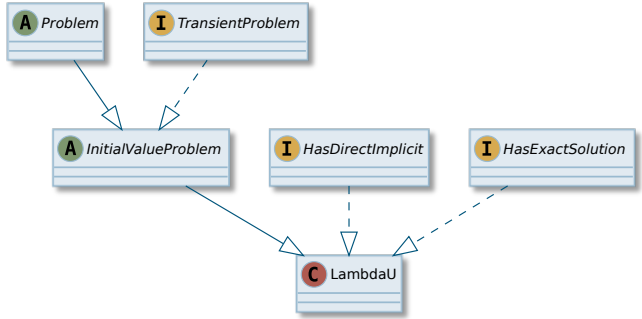
- interfaces for problem setups
- generic problem with specializations via mixins



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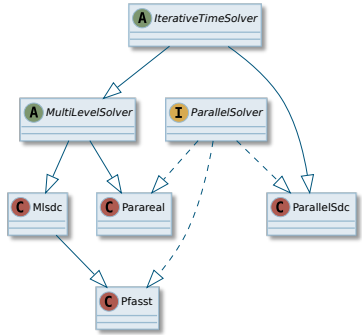
- interfaces for iterative time solvers
- providing generic building blocks of solvers



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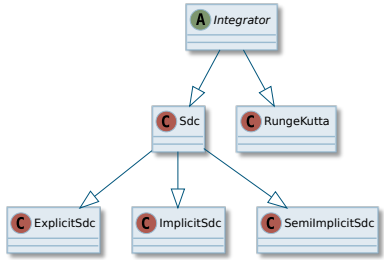
- abstract interface for integrators of ODEs
  e.g. *Runge-Kutta*, *Expl./Impl. Euler*, *SDC* etc.
- unified generic interface for executing integrator

  via method `.apply(*args, **kwargs)`



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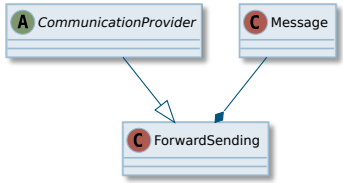
```

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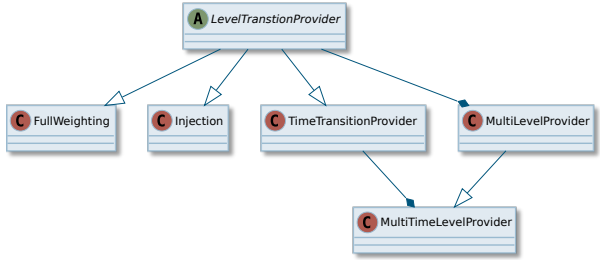
- abstract interface for generic level transitions
  e.g. *full weighting*, *injection*, *Lagrange-polynomial integration* etc.
- containers for multiple levels
  providing access to integrators of each level
- unified generic interface for transitions between levels
  via methods `.restrict(data, fine_id,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



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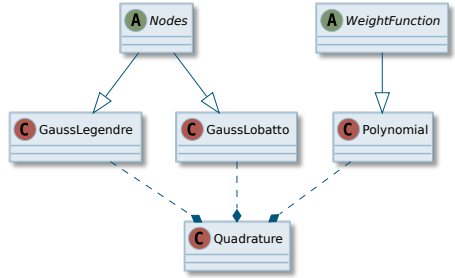
- providers of various quadrature nodes and weight functions
  e.g. Gauss-Lobatto, Gauss-Legendre, polynomial, etc.
- providers aggregated in basic quadrature interface
  for intuitive methods:
  `.q_matrix.apply(data)` and `.s_matrix.apply(data, target_node)`



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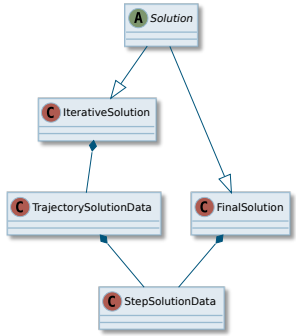
- containers for solution data + meta information
  e.g. time-node/step-wise, trajectory (consecutive time nodes)
- container interface for complete solutions
  e.g. only last time node of last iteration or all nodes of all iterations



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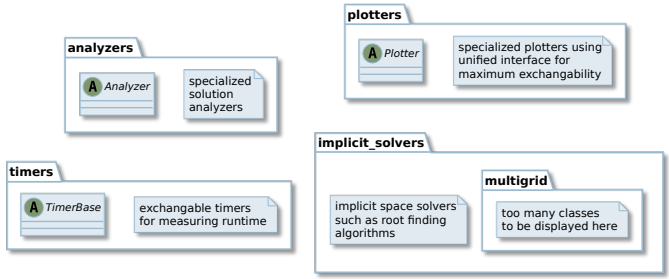

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Part III: Goals for PyPinT

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Goals for PyPinT

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

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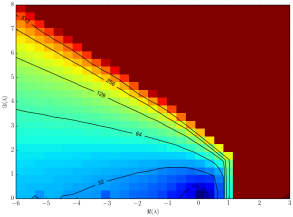
Part IV: Proof of Concept

May 28, 2014 | Torbjörn Klatt, Dieter Moser, Robert Speck

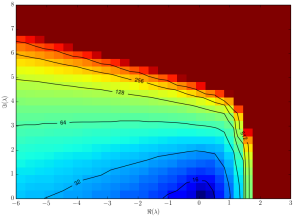
Implementation of SDC and MLSDC

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

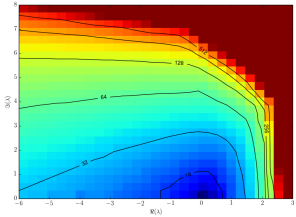
SDC



3 Gauss-Lobatto nodes



5 Gauss-Lobatto nodes



7 Gauss-Lobatto nodes

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.pyplt
```

Advantages of *PyPinT*

"towards" . . .

- 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)

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Thank you for your attention!

Questions?

(now or later)

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

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