

PyPinT

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

May 28, 2014 | Dieter Moser, Torbjörn Klatt, Dr. Robert Speck <{d.moser,t.klatt,r.speck}@fz-juelich.de> | 3rd Workshop on Parallel-in-Time Integration Methods

Overview

- 1 Recap of existing Parallel-in-Time Algorithms
- 2 The *PyPinT* Framework Explained
- 3 Goals
- 4 Proof of Concept — Examples Analyzed



PyPinT

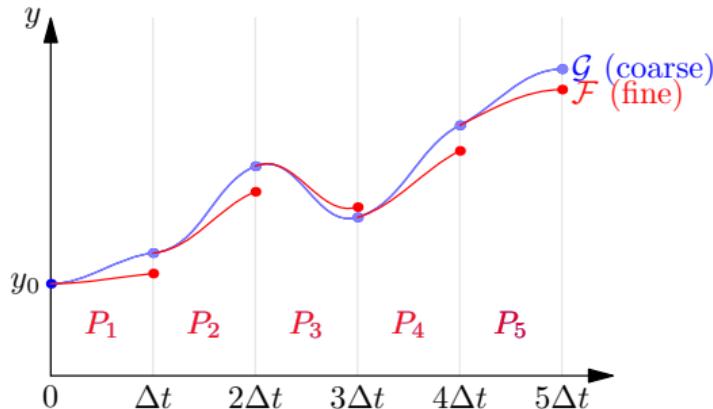
Part I: Existing Parallel-in-Time Approaches

May 28, 2014 | Dieter Moser, Torbjörn Klatt, Dr. Robert Speck <{d.moser,t.klatt,r.speck}@fz-juelich.de>

Parareal

Reference

- 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]

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

Integral Deferred Corrections

Reference

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

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

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

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

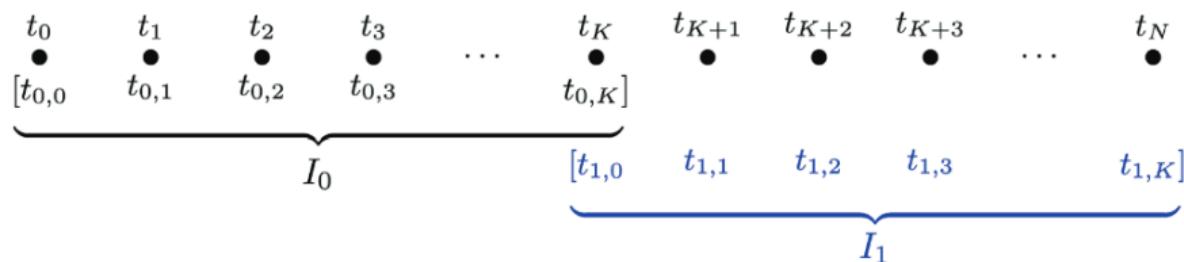
Revisionist IDC

Reference

One equation

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

different strategies of computation



What is needed? Integrator, Evaluation of F

Multilevel SDC

Reference

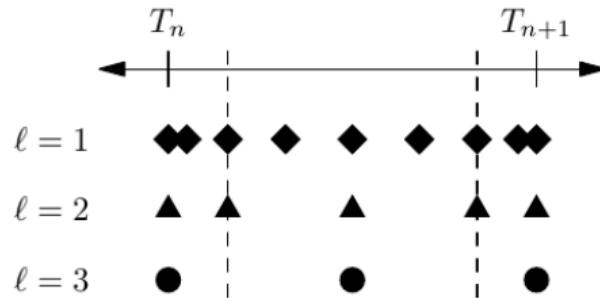
One equation

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

different strategies of computation

What is needed?

- Integrator
- Evaluation of F
- Interpolation
- Restriction



PFASST



PyPinT

Part II: The PyPinT Framework Explained

May 28, 2014 | Dieter Moser, Torbjörn Klatt, Dr. Robert Speck <{d.moser,t.klatt,r.speck}@fz-juelich.de>

Basic Concept

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



Modules

Abstract Modelling of PinT Algorithms

pypint

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

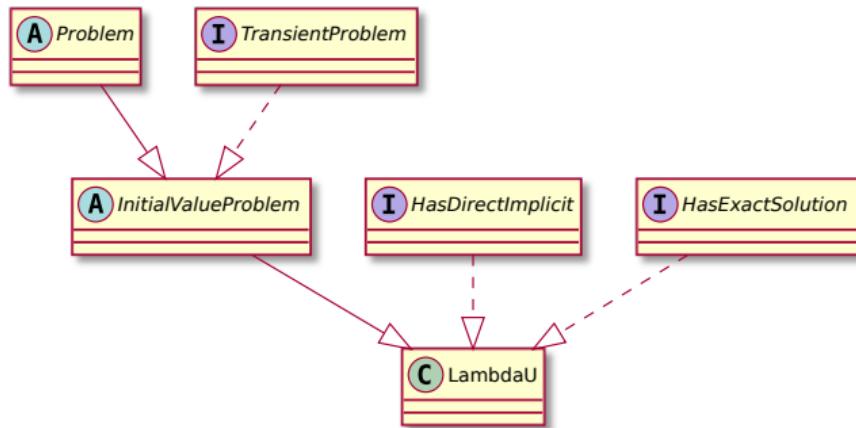


Modules

Abstract Modelling of PinT Algorithms

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

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



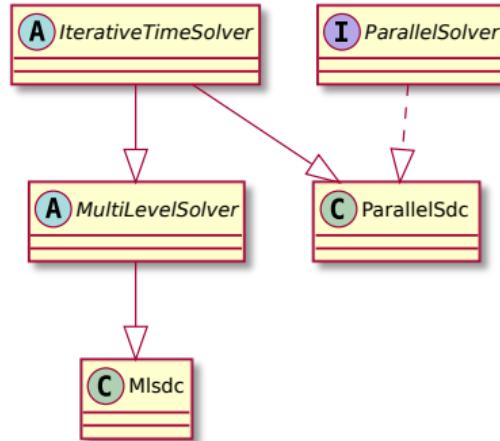
Modules

Abstract Modelling of PinT Algorithms

pypint

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

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



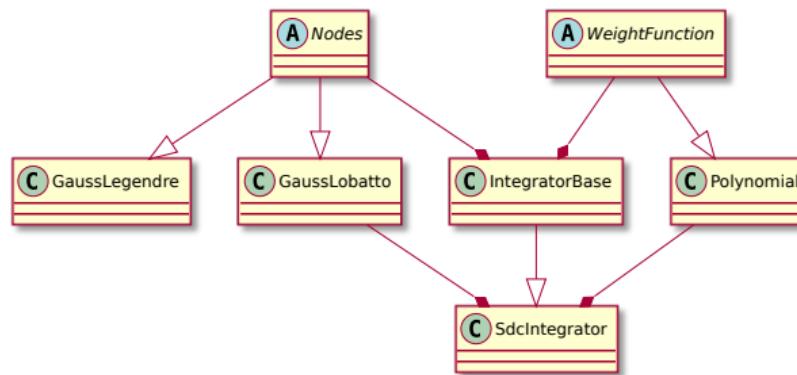
Modules

Abstract Modelling of PinT Algorithms

pypint

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

- providers of various quadrature nodes and weight functions
e.g. Gauss-Lobatto, Gauss-Legendre, polynomial, etc.
- providers aggregated in integrators
for intuitive `.integrate(data, from_node=0, to_node='last')` method



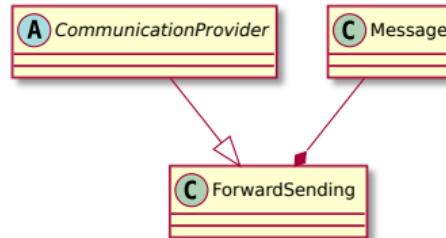
Modules

Abstract Modelling of PinT Algorithms

pypint

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

- 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



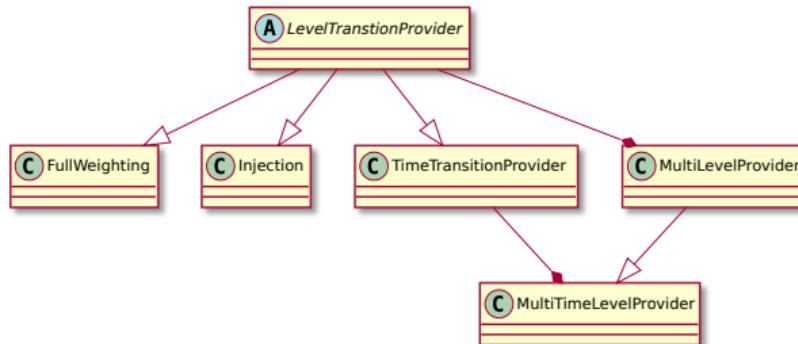
Modules

Abstract Modelling of PinT Algorithms

pypint

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

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



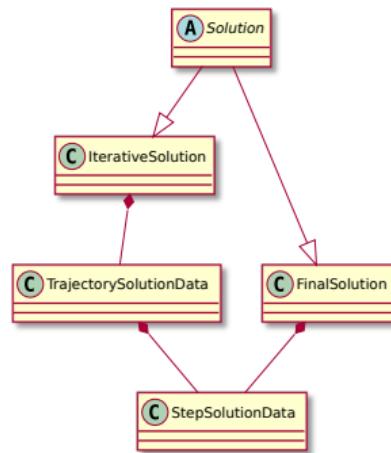
Modules

Abstract Modelling of PinT Algorithms

pypint

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

- 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



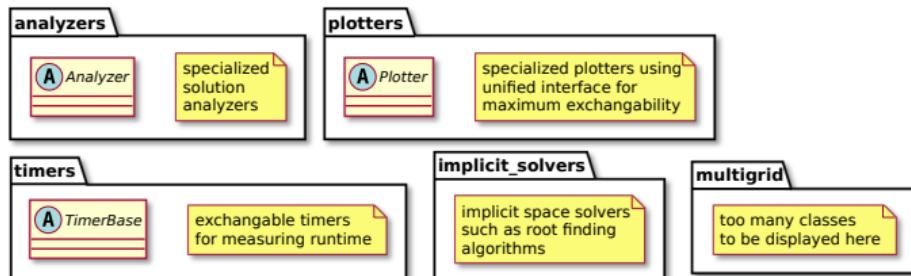
Modules

Abstract Modelling of PinT Algorithms

pypint

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

- 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





PyPinT

Part III: Goals for PyPinT

May 28, 2014 | Dieter Moser, Torbjörn Klatt, Dr. Robert Speck <{d.moser,t.klatt,r.speck}@fz-juelich.de>

Goals for PyPinT

- providing generic framework for PINT algorithms

Goals for PyPinT

- providing generic framework for PINT algorithms
⇒ easy comparability of different algorithms' building blocks

Goals for PyPinT

- providing generic framework for PINT algorithms
⇒ easy comparability of different algorithms' building blocks
- intuitive user-expandability through well-defined interfaces

Goals for PyPinT

- providing generic framework for PINT algorithms
⇒ easy comparability of different algorithms' building blocks
- intuitive user-expandability through well-defined interfaces
⇒ fast exchangability and prototyping of different building blocks

Goals for PyPinT

- providing generic framework for PINT algorithms
⇒ easy comparability of different algorithms' building blocks
- intuitive user-expandability through well-defined interfaces
⇒ fast exchangability and prototyping of different building blocks
- well-tested and well-documented implementations of PINT algorithms

Goals for PyPinT

- providing generic framework for PINT algorithms
⇒ easy comparability of different algorithms' building blocks
- intuitive user-expandability through well-defined interfaces
⇒ fast exchangability and prototyping of different building blocks
- well-tested and well-documented implementations of PINT algorithms
⇒ suited for educational use

Goals for PyPinT

- providing generic framework for PINT algorithms
⇒ easy comparability of different algorithms' building blocks
- intuitive user-expandability through well-defined interfaces
⇒ fast exchangability and prototyping of different building blocks
- well-tested and well-documented implementations of PINT algorithms
⇒ suited for educational use
- open-source hosted on  GitHub

Goals for PyPinT

- providing generic framework for PINT algorithms
⇒ easy comparability of different algorithms' building blocks
- intuitive user-expandability through well-defined interfaces
⇒ fast exchangability and prototyping of different building blocks
- well-tested and well-documented implementations of PINT algorithms
⇒ suited for educational use
- open-source hosted on  GitHub
⇒ reaching young & rising developers and scientists promoting PINT algorithms



PyPinT

Part IV: Proof of Concept

May 28, 2014 | Dieter Moser, Torbjörn Klatt, Dr. Robert Speck <{d.moser,t.klatt,r.speck}@fz-juelich.de>

Thank you for your attention!

Questions?

(now or later)

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

Dieter Moser
Juelich Supercomputing Centre
Building 16.3, Room 022
Tel: +49 2461 61 96453
eMail: d.moser@fz-juelich.de

Torbjörn Klatt
Juelich Supercomputing Centre
Building 16.3, Room 022
Tel: +49 2461 61 96452
eMail: t.klatt@fz-juelich.de

Dr. Robert Speck *
Juelich Supercomputing Centre
Building 16.3, Room 131
Tel: +49 2461 61 1644
eMail: r.speck@fz-juelich.de

* corresponding author