JÜLICH
FORSCHUNGSZENTRUM

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

JÜLICH
FORSCHUNGSZENTRUM

PyPinT

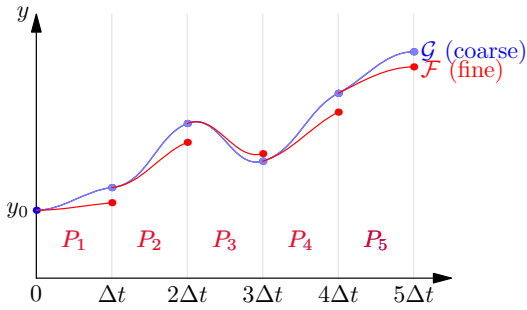
Part I: Existing Parallel-in-Time Approaches

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]

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

IDC and DC

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

Using the residual

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

to compute the error

$$e'(t) = f(t, \tilde{u} + e) - f(t, \tilde{y}) + r'(t)$$
$$e(0) = 0$$

for the next update

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

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

Using the residual

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

to compute the error

$$e'(t) = f(t, \tilde{u} + e) - f(t, \tilde{y}) + r'(t)$$
$$e(0) = 0$$

for the next update

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

RIDC

RIDC

PFASST

JÜLICH
FORSCHUNGSZENTRUM

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

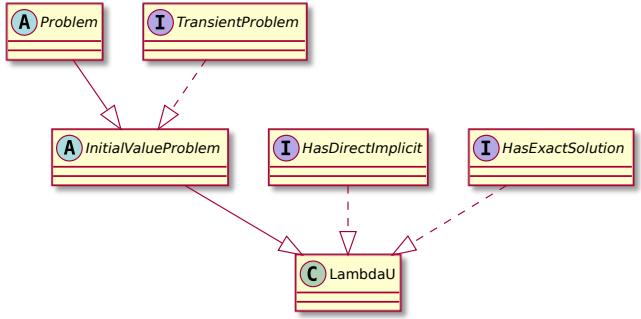
```
pypint
  ~.problems
  ~.solvers
  ~.integrators
  ~.communicators
  ~.multi_level_providers
  ~.solutions
  ~.plugins
```

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

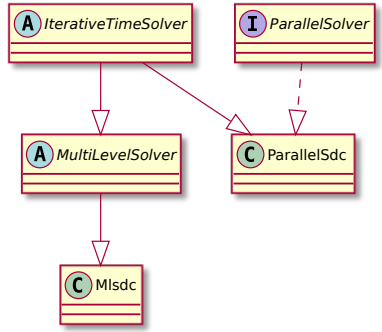


Modules

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

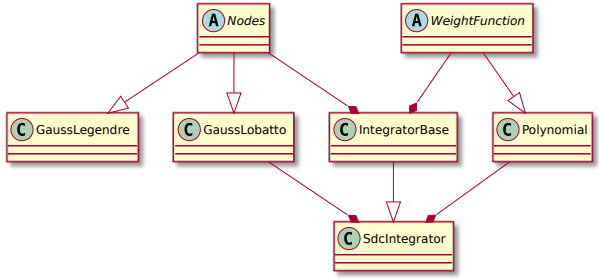


Modules

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

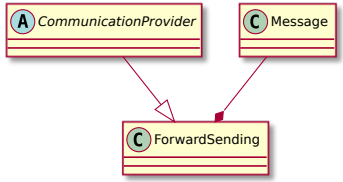


Modules

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

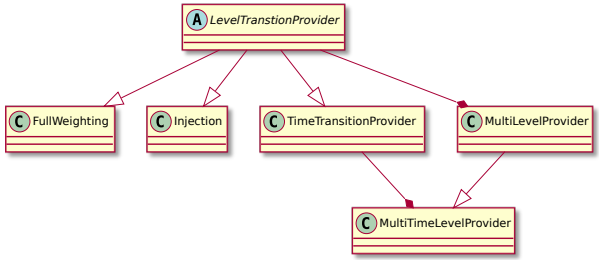


Modules

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)`

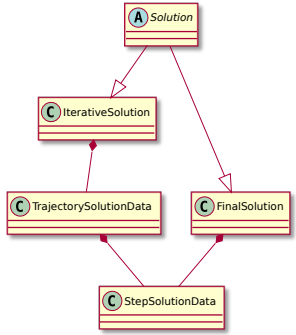


Modules

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

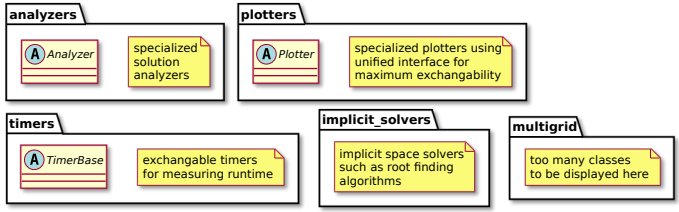


Modules

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



JÜLICH
FORSCHUNGSZENTRUM

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
  $\Rightarrow$ easy comparability of different algorithms' building blocks

Goals for PyPinT

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

Goals for PyPinT

- providing generic framework for PINT algorithms
  $\Rightarrow$ easy comparability of different algorithms' building blocks

- intuitive user-expandability through well-defined interfaces
  $\Rightarrow$ fast exchangability and prototyping of different building blocks

Goals for PyPinT

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

Goals for PyPinT

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

Goals for PyPinT

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

JÜLICH
FORSCHUNGSZENTRUM

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