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Parallel-in-time integration with PFASST

Swiss Numerical Analysis Day 2015

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Joint work with

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A fundamental turn toward concurrency

- In about 10 years, **Exascale** systems will require 100-million way parallelism
- Multitude of challenges for numerical methods:
  1. massive concurrency
  2. resilience against faults
  3. energy consumption
  4. ...

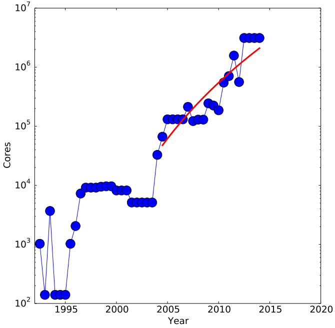


Figure: Number of cores in the top system in `www.top500.org`.

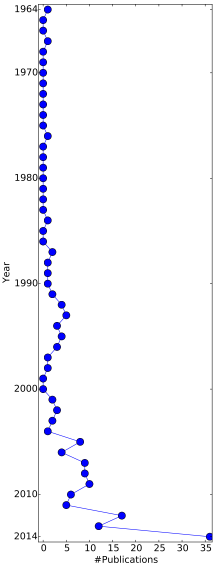
#8: Don't rethink your algorithms.
(K. Yelick, "Ten ways to waste a parallel computer", 2009)

51 years of parallel-in-time integration[1]

Parallelization in time can

1. extend strong scaling limits of space parallelization
2. help with the "trap of weak scaling"

- Interpolation-based approach (Nievergelt 1964)
- Parabolic or time multi-grid (Hackbusch 1984) and (Horton 1992)
- Parallel Runge-Kutta methods (e.g. Butcher 1997) and extrapolation (Richardson 1910)
- Parareal (Lions, Maday, Turinici 2001) and PITA (Farhat, Chandesris 2003)
- PFASST (Emmett, Minion 2012)
- MGRIT (Falgout et al. 2014)
- DG time multi-grid (Gander, Neumueller 2014)



[1] For a recent overview see M. Gander's paper.

Collocation

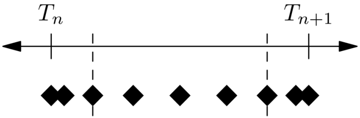


Figure: A time-step $[T_n, T_{n+1}]$ with $M = 9$ Gauss-Lobatto collocation nodes t_j.

Integrate initial value problem $u'(t) = f(u(t), t)$ from T_n to T_{n+1}:

- Consider Picard formulation of IVP

$$u(T_{n+1}) = u(T_n) + \int_{T_n}^{T_{n+1}} f(\tau, u(\tau))\ d\tau$$

- The integral is approximated by quadrature

$$\int_{T_n}^{T_{n+1}} f(\tau, u(\tau))\ d\tau \approx \Delta t \sum_{j=1}^{M} q_{n,j} f(t_j, u_j), \quad \text{with stages } u_j \in \mathbb{R}^N$$

- Collocation problem can compactly be written as

$$\mathbf{U} = \mathbf{U}_0 + \Delta t \mathbf{QF}(\mathbf{U}),\ \mathbf{U} = (u_1, \dots, u_M)^{\mathrm{T}} \in \mathbb{R}^{NM \times NM}$$

Richardson or discrete Picard iteration

- Rewrite the **collocation** equation as linear[1] equation

$$\mathbf{MU} = (\mathbf{I} - \Delta t\mathbf{QF})\,\mathbf{U} = \mathbf{U}_0$$

- Richardson iteration corresponds to (discrete) **Picard iteration**

$$\mathbf{U}^{k+1} = \mathbf{U}^k + \left(\mathbf{U}_0 - \mathbf{MU}^k\right) = \mathbf{U}_0 + \Delta t\mathbf{QFU}^k \approx u_0 + \int_{T^n}^{T^{n+1}} f(\tau, u^k(\tau))\ d\tau$$

$\rightarrow$ Typically not very good convergence properties

- Need a **preconditioner** $\mathbf{Q}_\Delta$ with

$$\Delta t\mathbf{Q}_\Delta\mathbf{FU} \approx \Delta t\mathbf{QFU} \approx \int_{T_n}^{T_{n+1}} f(u(s))\ ds$$

which is easy to invert

[1] For the sake of simplicity

Spectral deferred corrections (SDC)

Dutt, Greengard, Rokhlin
BIT Numerical Mathematics 2000

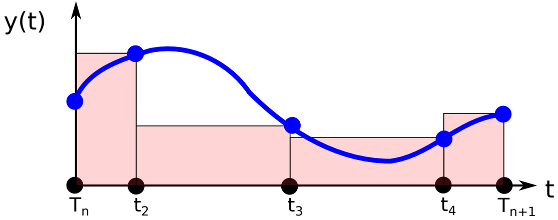


Figure: Use composite rectangular rule $\mathbf{Q}_\Delta$ to precondition high-order collocation rule $\mathbf{Q}$

- Consider preconditioned Richardson iteration

$$\mathbf{Y}^{k+1} = \mathbf{Y}^k + (\mathbf{I} - \Delta t \mathbf{Q}_\Delta \mathbf{F})^{-1} \left[\mathbf{Y}_0 - (\mathbf{I} - \Delta t \mathbf{Q}\mathbf{F}) \mathbf{Y}^k \right], \quad \mathbf{Q}_\Delta \approx \mathbf{Q}, \quad \mathbf{Y} \in \mathbb{R}^{NM}$$

- Can computes this node-by-node which gives "classical" SDC sweep

$$y_m^{k+1} = y_{m-1}^{k+1} + \Delta t f(y_m^{k+1}) - \Delta t f(y_m^k) + \sum_{j=1}^{M} s_{m,j} f(y_j^k), \quad y_m^k \in \mathbb{R}^N$$

- Classically SDC is derived from error/correction equations (Dutt et al. 2000)

Multi-level spectral deferred corrections (MLSDC)

Speck, Ruprecht, Emmett, Minion, Bolten, Krause

BIT Numerical Mathematics 2014

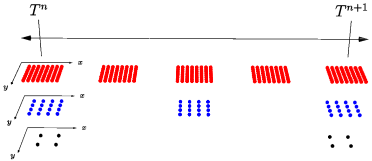


Figure: Hierarchy of three levels with 5 (red), 3 (blue) and 2 (black) collocation nodes and a coarsened spatial mesh for MLSDC applied to a semi-discrete time-dependent PDE.

- SDC sweeps on a **hierarchy** of levels
  $\rightarrow$ SDC sweep analogue to relaxation in space MG
- Employ **FAS correction** to accurately represent solution on $l > 1$
- Reduce overhead from f evaluations on higher levels by **coarsening**:
  $\rightarrow$ reduced number of points, reduced order, reduced implicit solves, reduced physics, ...

PFASST

Emmett, Minion

CAMCOS 2012

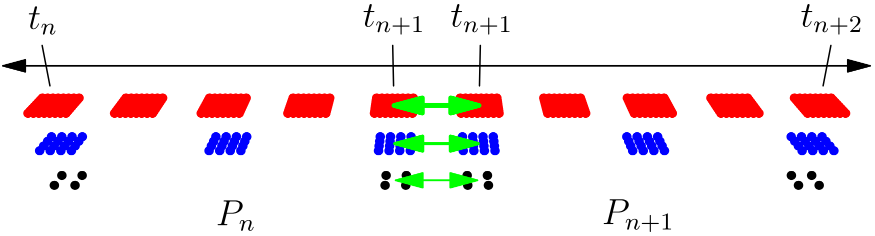


Figure: PFASST performs MLSDC cycles concurrently on multiple time steps, sending updated initial values after every sweep.

PFASST in massively parallel simulations

- Particle based Navier-Stokes solver on $262,144$ cores[1]
- Mesh-based combination with parallel multi-grid on $458,752$ cores[2]

[1] Speck et al., Supercomputing 2012

[2] Ruprecht et al., Supercomputing 2013

Inexact SDC

Speck, Ruprecht, Emmett, Minion, Krause
LNCSE 2015

Algorithm 1: Standard SDC sweep

```
while (sdc_residual > time_tolerance) do
    for (m = 1 ... #substeps) do
        while (pmg_residual > space_tolerance) do
            Perform PMG V-cycle
        end
        Perform backward Euler step: y^k_{m-1} → y^k_m
    end
end
```

Algorithm 2: Sweep with inexact SDC

```
while (sdc_residual > time_tolerance) do
    for (m = 1 ... #substeps) do
        // Incomplete implicit solve
        for (k = 1 ... NumV) do
            Perform PMG V-cycle
        end
        Perform approximate backward Euler step: y^k_{m-1} → y^k_m
    end
end
```

IPFASST convergence

Minion et al.
SISC 2015

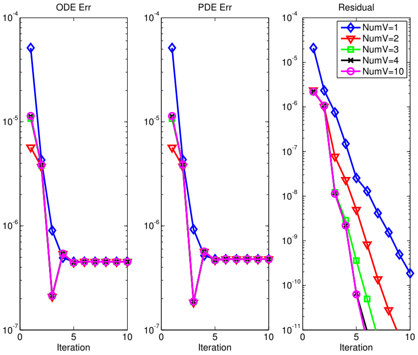


Figure: Convergence of IPFASST for simple $u_t = u_{xx}$ problem depending on number of V-cycles.

- Stage y_m^k becomes increasingly accurate initial guess when solving for y_m^{k+1}:

$$y_m^{k+1} = y_{m-1}^{k+1} + \Delta t f(y_m^{k+1}) - \Delta t f(y_m^k) + \sum_{j=1}^{M} s_{m,j} f(y_j^k), \quad y_m^k \in \mathbb{R}^N$$

IPFASST strong scaling

Minion et al.

SISC 2015

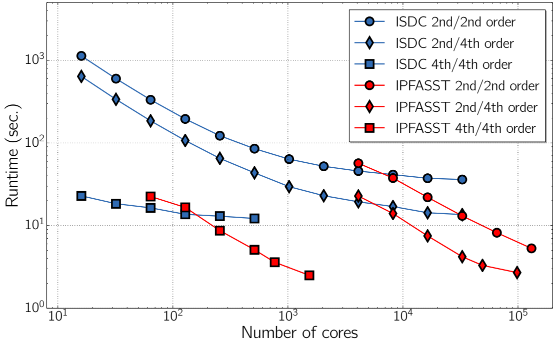


Figure: Strong scaling of IPFASST with parallel multi-grid solver (PMG) on the IBM Blue Gene/Q JUQUEEN at JSC. All shown runs provide the same accuracy.

- Space parallelization through parallel multigrid (code by M. Bolten)
- IPFASST can provide speedup beyond saturation of spatial parallelization alone

Summary

- SDC is a preconditioned fixed point iteration to solve collocation equation
- MLSDC is multi-level extension with sweeps in a sense analogue to relaxation
- PFASST parallelizes MLSDC in time by iterating concurrently on multiple time-steps
- Iterative structure of SDC provides increasingly accurate starting values for PMG
  $\rightarrow$ can use approximate solves in implicit sub steps
  $\rightarrow$ corresponds to different order of time and space sweeps/cycles
- Results in ISDC, IMLSDC, IPFASST
- IPFASST shows good parallel performance on $\mathcal{O}(10k - 100k)$ cores in first benchmarks

The End – for now.