Rethinking HPC algorithms for Exascale: the case for Adjoint Computations

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Scheduling 102,
Scheduling under constraints

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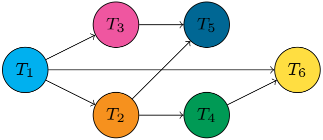
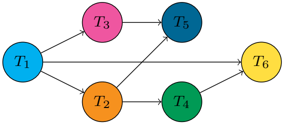
Scheduling

- p processors (or nodes or cores or computing units).
- An application represented by a DAG $\mathcal{G} = (V, E)$:
  - Vertices are tasks (or functions to be computed)
  - Edges represent data dependency (need to be respected)



Motivational example



Assume tasks have unit size and there are two processors.

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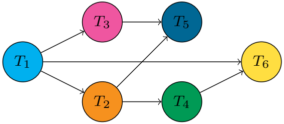

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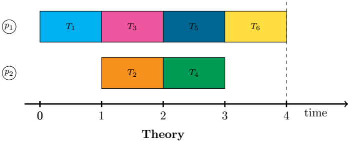
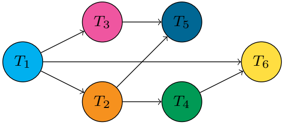


- In theory, optimal schedule ☺

Motivational example



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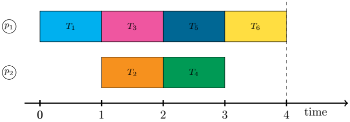
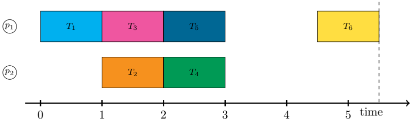


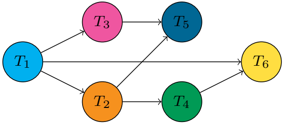
Theory



Practice

- In theory, optimal schedule ☺
- In practice, not what we expected ☹.

Motivational example



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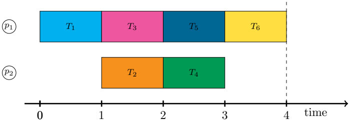

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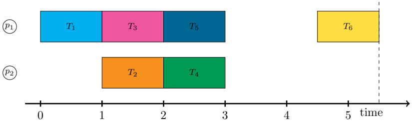
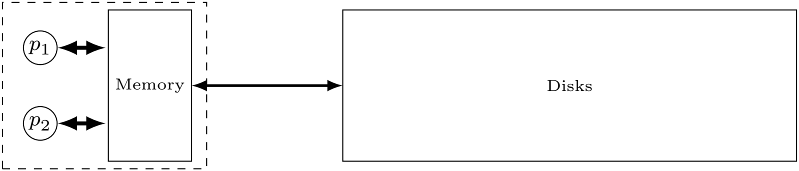


Practice

- In theory, optimal schedule ☺
- In practice, not what we expected ☹.

What happened?

Data is critical

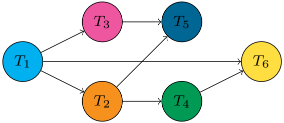


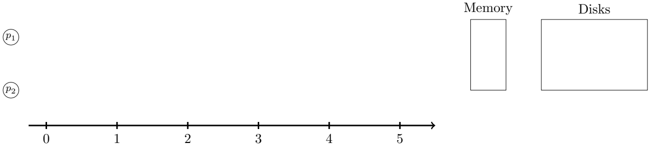
Overview of a computer.

In general,

- Memory is small but accesses are fast;
- Disks are large but accesses are slow.

Back to our schedule





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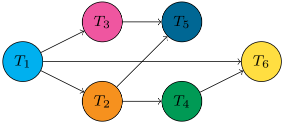

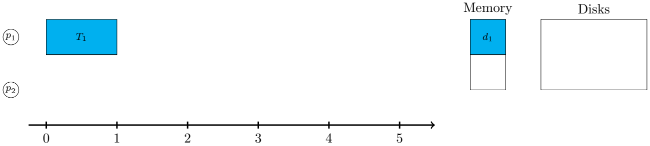

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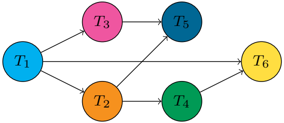

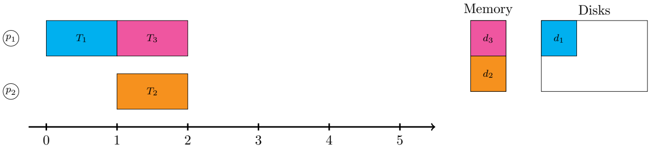

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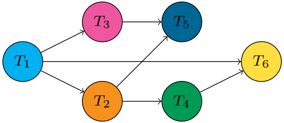

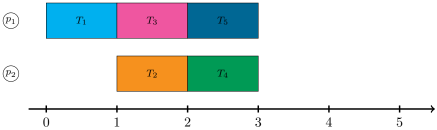

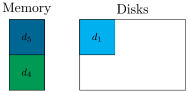

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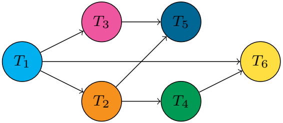

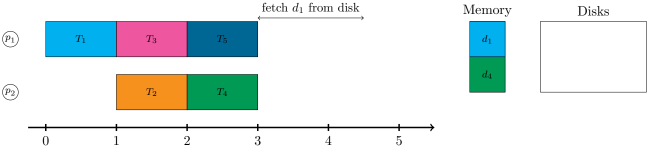

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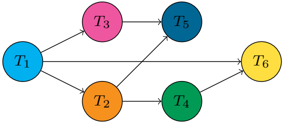

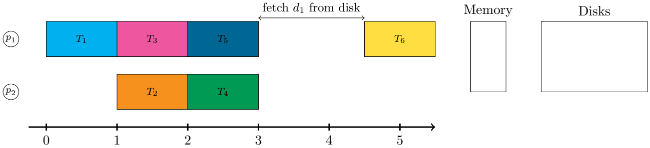

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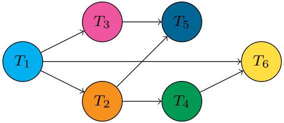

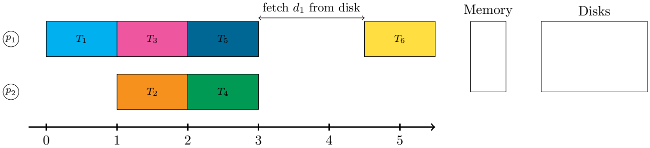

Can we do better (or prove that we cannot)?

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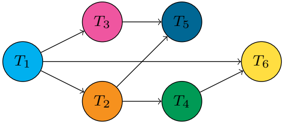

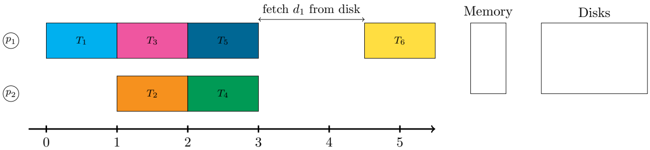

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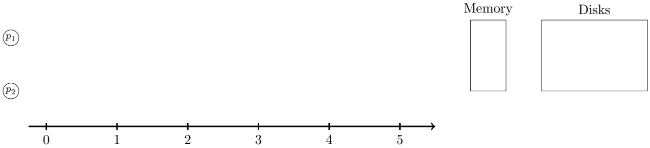

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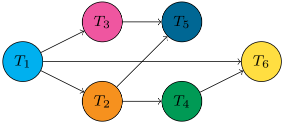

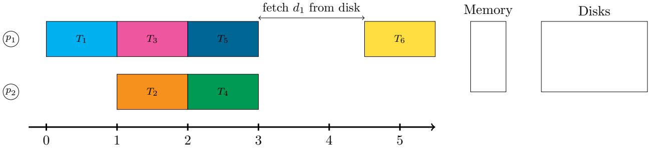

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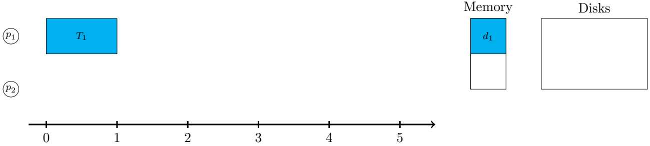

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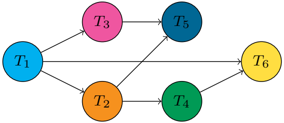

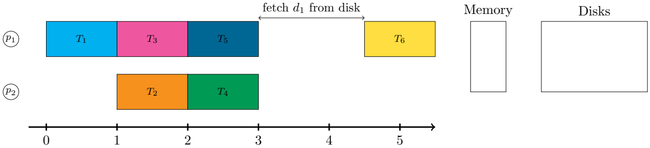

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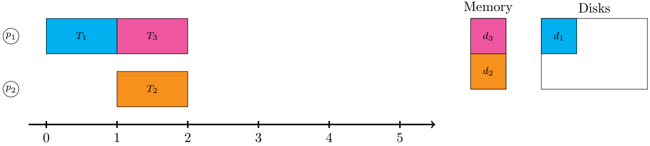

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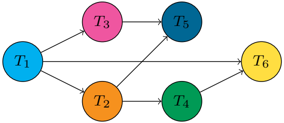

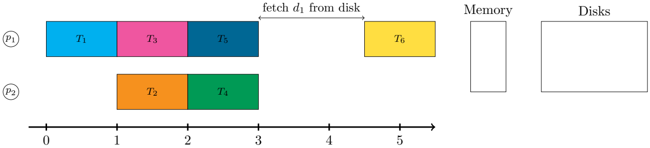

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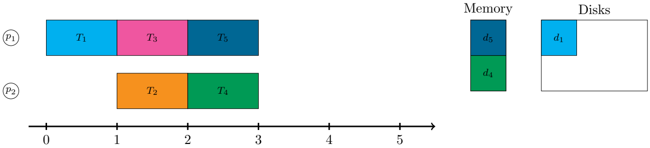

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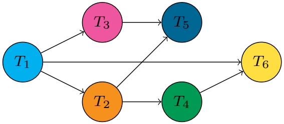

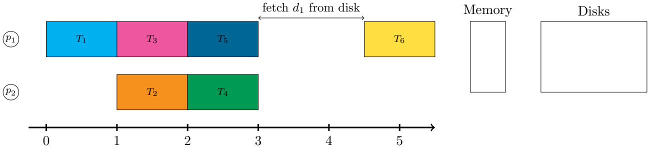

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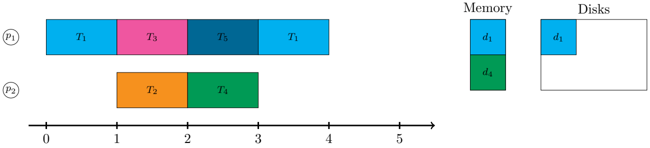

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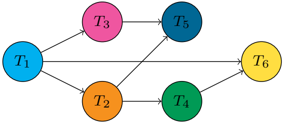

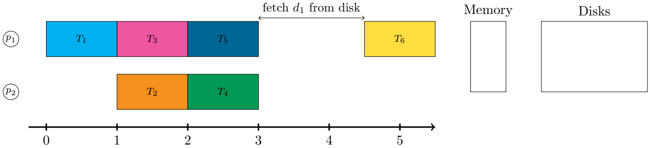

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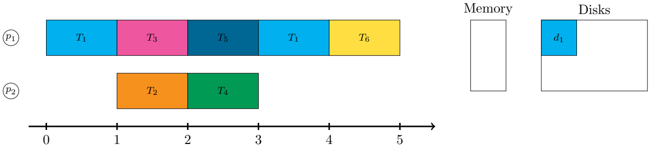

Some numbers

(Brief) history of supercomputers at Argonne National Lab:

	Intrepid	Mira
Year	2008-2013	2013-
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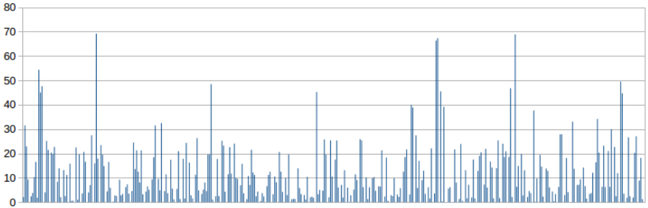

Analysis of the Intrepid system @Argonne: I/O throughput decrease (percentage per application, over 400 applications).

What next

Some directions to solve this problem:

- Better I/O Management?
- Rethinking I/O intensive applications:
  from computation-oriented thinking to I/O-oriented thinking.

Optimal multistage algorithms for adjoint computation

Guillaume Aupy,
work with Julien Herrmann, Paul Hovland & Yves Robert

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Ice-sheet model (I)

"In climate modelling, Ice-sheet models use numerical methods to simulate the evolution, dynamics and thermodynamics of ice sheets." (wikipedia)

Model Algorithm (single timestep)

1. Evaluate driving stress $\tau_d = \rho g h \nabla s$
2. Solve for velocities

   DO i = 1, max_iter

   i. Evaluate nonlinear viscosity v_i from iterate $\boldsymbol{u}_i$

   ii. Construct stress matrix $A\{v_i\}$

   iii. Solve linear system $A\ \boldsymbol{u}_{i+1} = \tau_d$

   iv. (Exit if converged)

   ENDDO
3. Evolve thickness (continuity eqn)

Automatic differentiation (AD) tools generate code for adjoint of operations

Credit: Daniel Goldberg

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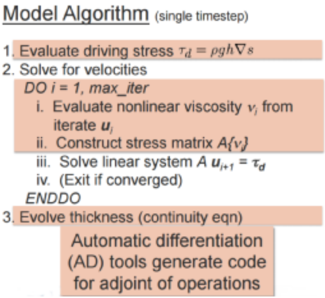

Simpler Version:

proc Model Algorithm($u_0, \boldsymbol{y}$)
begin
  Do stuff;
  for $i = 0$ *to* n **do**
    $u_{i+1} = f_i(u_i)$;
    Do stuff;
  end
  /* $F(u_0) = f_n \circ f_{n-1} \circ \ldots \circ f_0(u_0)$ */
  Compute $\boldsymbol{\nabla} F(u_0)\boldsymbol{y}$;
end

Credit: Daniel Goldberg

Ice-sheet model (II)

$$F(u_0) = f_n \circ f_{n-1} \circ \ldots \circ f_1 \circ f_0(u_0)$$

$$\begin{aligned} \boldsymbol{\nabla} F(u_0)\boldsymbol{y} &= Jf_0(u_0)^T \cdot \boldsymbol{\nabla}(f_n \circ f_1)(u_1) \cdot \boldsymbol{y} \\ &= \boxed{Jf_0(u_0)^T \cdot Jf_1(u_1)^T \cdot \ldots \cdot Jf_{n-1}(u_{n-1})^T \cdot Jf_n(u_n)^T \cdot \boldsymbol{y}} \end{aligned}$$

$$\begin{aligned} Jf^T &= \text{ Transpose Jacobian matrix of } f; \\ u_{i+1} &= f_i(u_i) = f_i\left(f_{i-1} \circ \ldots \circ f_0(u_0)\right). \end{aligned}$$

Ice-sheet model (II)

$$F(u_0) = f_n \circ f_{n-1} \circ \ldots \circ f_1 \circ f_0(u_0)$$

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But then, isn't there a faster algorithm?

A better solution?

$$\boldsymbol{\nabla} F(u_0)\boldsymbol{y} = Jf_0(u_0)^T \cdot Jf_1(u_1)^T \cdot \ldots \cdot Jf_{n-1}(u_{n-1})^T \cdot Jf_n(u_n)^T \cdot \boldsymbol{y}$$

```
proc Algo A(u_0, y)
begin
    Do stuff;
    for i = 0 to n do
        u_{i+1} = f_i(u_i);
        Do stuff;
    end
    Compute ∇F(u_0)y;
end
```

```
proc Algo B(u_0, y)
begin
    Do stuff;
    for i = 0 to n do
        u_{i+1} = f_i(u_i);
        Do stuff;
        v_{i+1} = v_i · Jf_{i+1}(u_{i+1})^T;
    end
end
```

A better solution?

$$\nabla F(u_0)\boldsymbol{y} = Jf_0(u_0)^T \cdot Jf_1(u_1)^T \cdot \ldots \cdot Jf_{n-1}(u_{n-1})^T \cdot Jf_n(u_n)^T \cdot \boldsymbol{y}$$

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    end
end
```

What is the problem with Algo B?

A BETTER SOLUTION?

$$\nabla F(u_0)\boldsymbol{y} = Jf_0(u_0)^T \cdot Jf_1(u_1)^T \cdot \ldots \cdot Jf_{n-1}(u_{n-1})^T \cdot Jf_n(u_n)^T \cdot \boldsymbol{y}$$

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proc Algo B(u_0, y)
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        Do stuff;
        v_{i+1} = v_i · Jf_{i+1}(u_{i+1})^T;
    end
end
```

What is the problem with Algo B?

$$\nabla F(u_0)\boldsymbol{y} = \left(\left(\ldots\left(Jf_0{}^T \cdot Jf_1{}^T\right) \cdot \ldots \cdot Jf_{n-1}{}^T\right) \cdot Jf_n{}^T\right) \cdot \boldsymbol{y} \quad n \text{ MatMat ops}$$

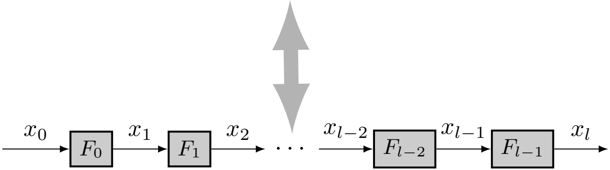
$$\nabla F(u_0)\boldsymbol{y} = Jf_0{}^T \cdot \left(Jf_1{}^T \cdot \ldots \cdot \left(Jf_{n-1}{}^T \cdot \left(Jf_n{}^T \cdot \boldsymbol{y}\right) \ldots\right)\right) \quad n \text{ MatVec ops}$$

Adjoint computation

$$\begin{aligned} F_i(x_i) &= x_{i+1} \quad && i < l \\ \bar{F}_i(x_i, \bar{x}_{i+1}) &= \bar{x}_i && i \le l \end{aligned}$$

Adjoint computation

$$\boldsymbol{F_i(x_i) = x_{i+1} \quad i < l}$$
$$\bar{F}_i(x_i, \bar{x}_{i+1}) = \bar{x}_i \qquad i \leq l$$



Adjoint computation

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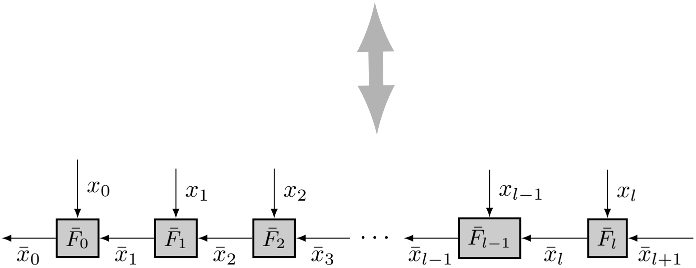
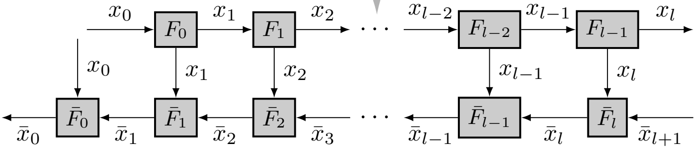


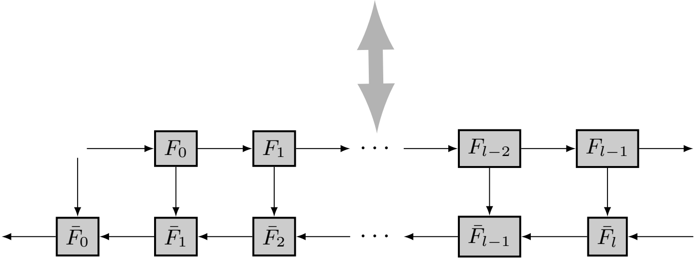
Adjoint computation

$$
\begin{aligned}
F_i(x_i) &= x_{i+1} \quad & i < l \\
\bar{F}_i(x_i, \bar{x}_{i+1}) &= \bar{x}_i \quad & i \leq l
\end{aligned}
$$

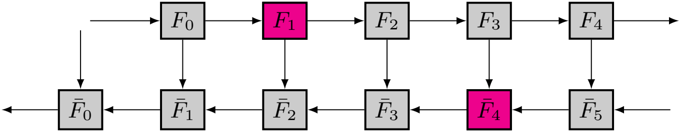


Adjoint computation

$$\begin{aligned} F_i(x_i) &= x_{i+1} & i < l \\ \bar{F}_i(x_i, \bar{x}_{i+1}) &= \bar{x}_i & i \le l \end{aligned}$$



Model of Computation



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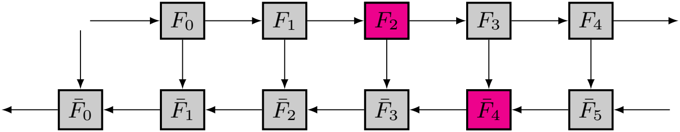

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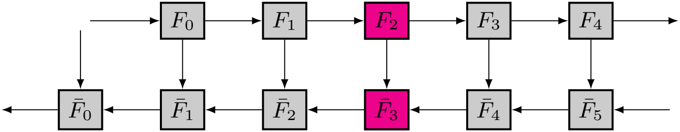

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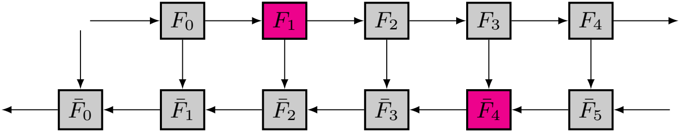

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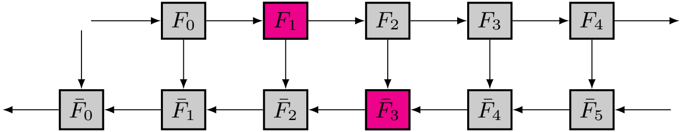

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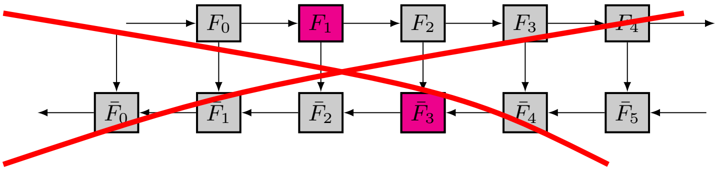

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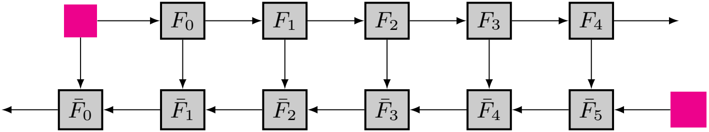

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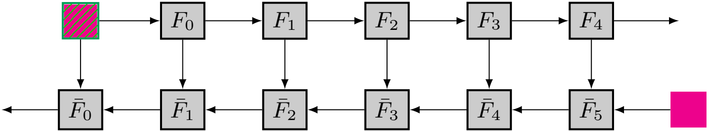

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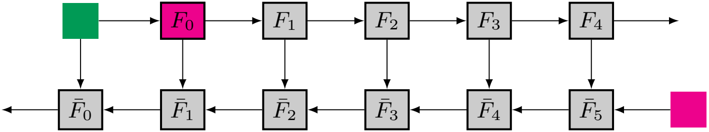

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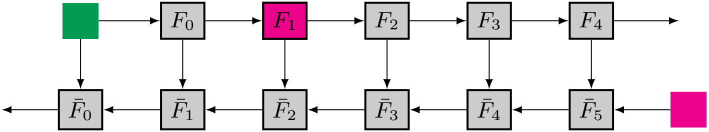

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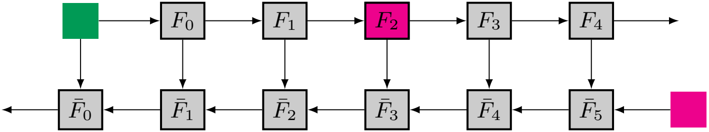

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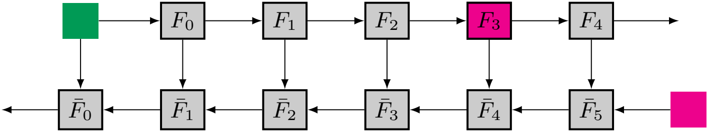

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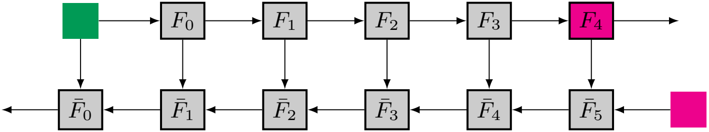

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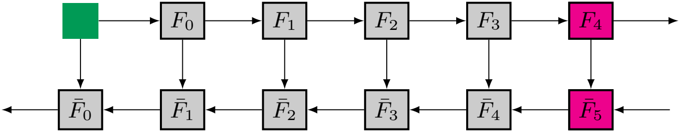

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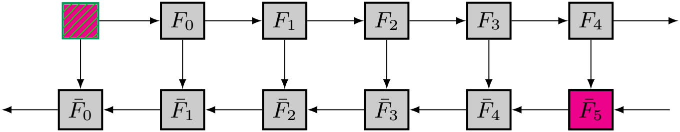

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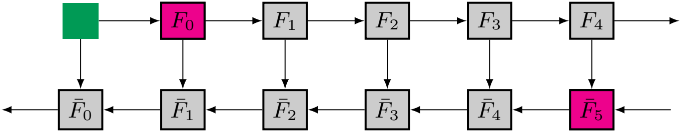

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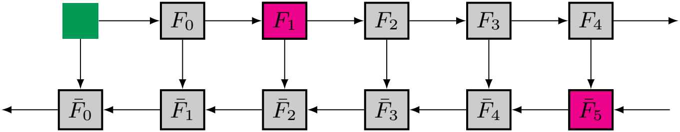

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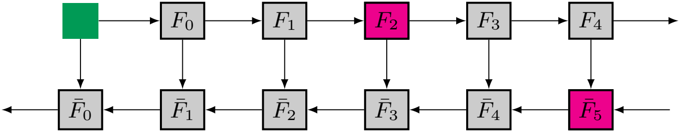

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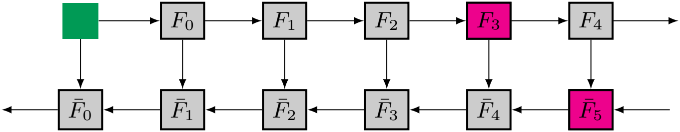

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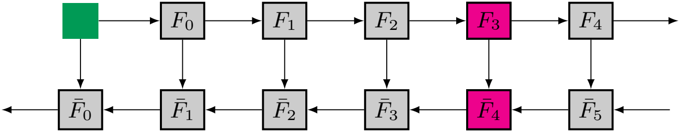

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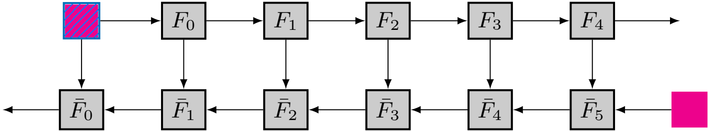

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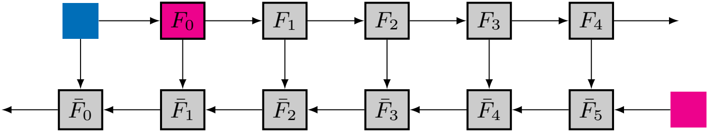

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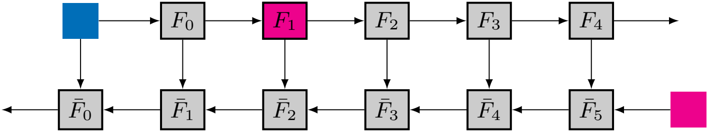

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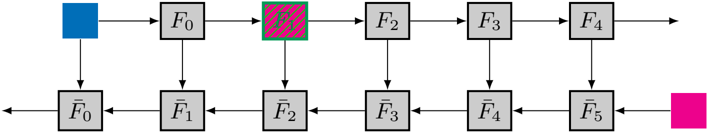

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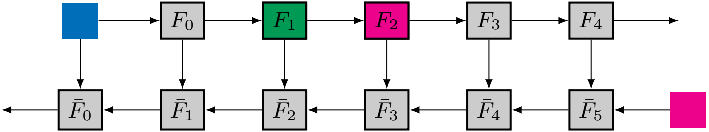

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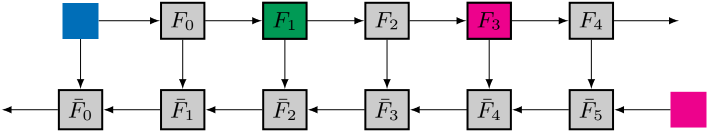

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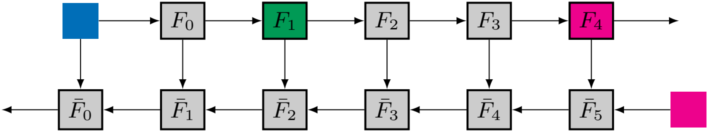

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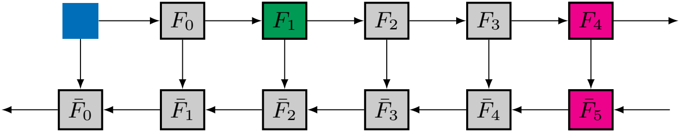

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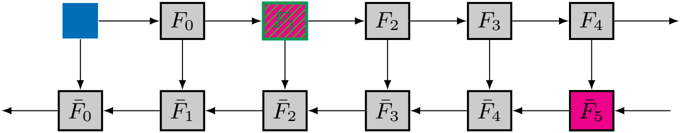

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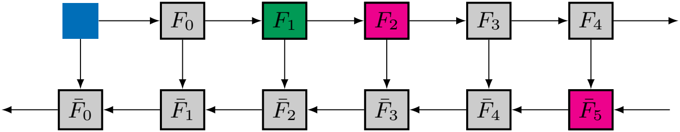

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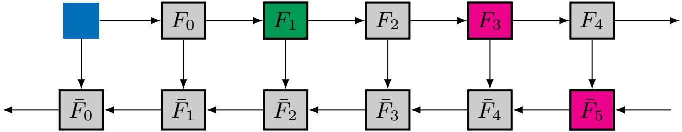

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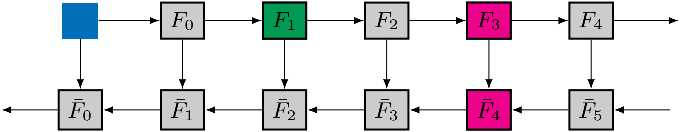

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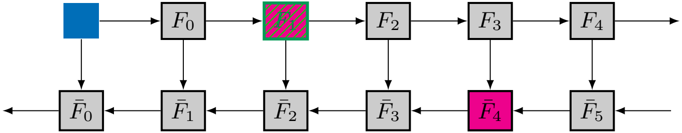

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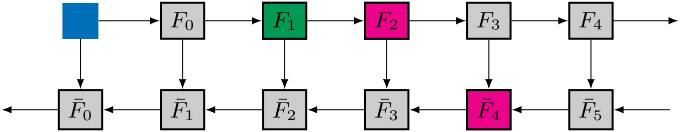

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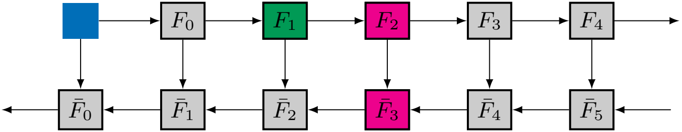

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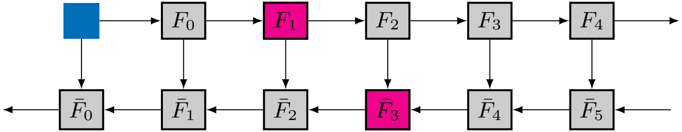

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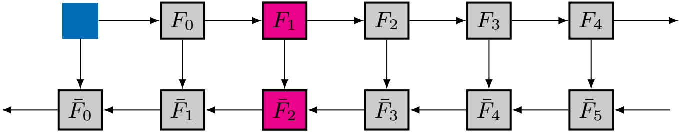

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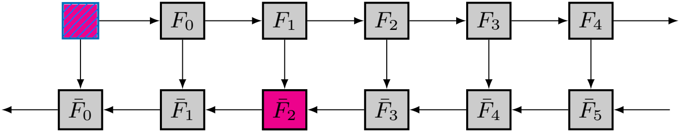

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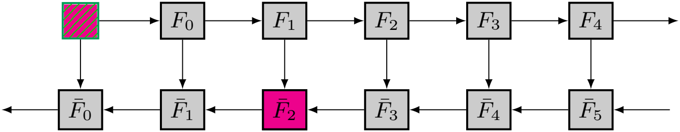
  - Cost to write: w_d,
  - Cost to read: r_d.

Model of Computation



- Two buffers: store output of computations (x_i or $\bar{x}_i$). Initial state: contains x_0 and $\bar{x}_{l+1}$.
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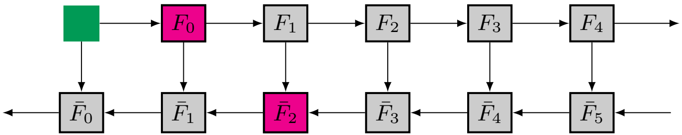

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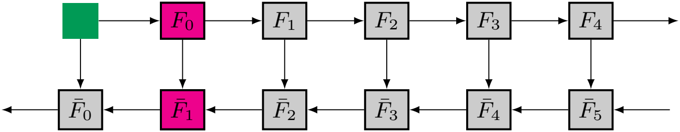

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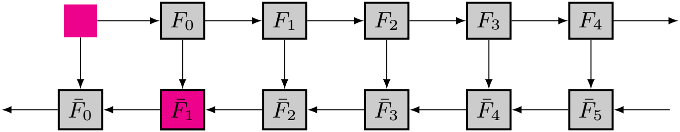

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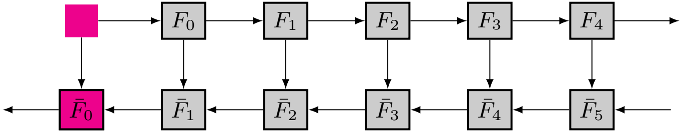

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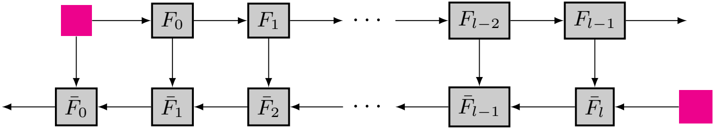
Problem formulation

We want to minimize the makespan of:

		Initial state:
AC graph:	size l	
Steps:	u_f, u_b	
Memory:	c_m, $w_m = r_m = 0$,	$\mathcal{M}_{\text{ini}} = \emptyset$
Disks:	$c_d = +\infty, w_d, r_d,$	$\mathcal{D}_{\text{ini}} = \emptyset$
Buffers:	$\mathcal{B}^{\top}$, $\mathcal{B}^{\perp}$	$\mathcal{B}^{\top}_{\text{ini}} = \{x_0\}$, $\mathcal{B}^{\perp}_{\text{ini}} = \{\bar{x}_{l+1}\}$



GW00: Revolve(l, c_m), optimal algorithm with c_m memory slots and no disk slots.

SW09: SWA*, an algorithm based on Revolve that takes disk storage into acount.

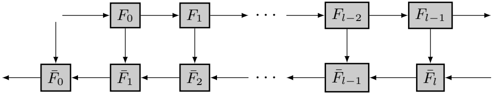
(i) $\mathrm{SWA}(l, c_m, c_d, w_d, r_d) \approx \textsc{Revolve}(l, c_d + c_m)$[1]

(ii) $\mathrm{SWA}^\star(l, c_m, w_d, r_d) = \min_{c_d=0\ldots l-c_m} \mathrm{SWA}(l, c_m, c_d, w_d, r_d)$

This work: optimal algorithm with disk storage.

[1] out of the $c_d + c_m$ slots used by Revolve, the c_d slots the least used are considered disk slots.

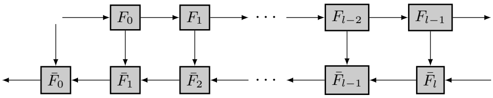
A grasp of the proof



Any algorithm works in two phases:

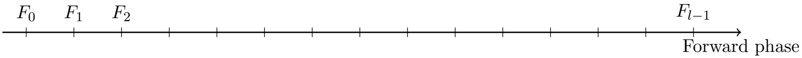
- The forward phase (before executing $\bar{F}_l$);
- The backward phase (that starts when executing $\bar{F}_l$);

The forward phase

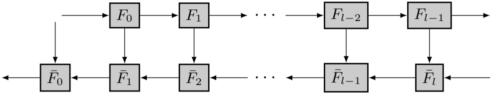


In this phase:

- We execute all F-operations;

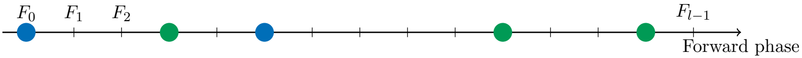


The forward phase

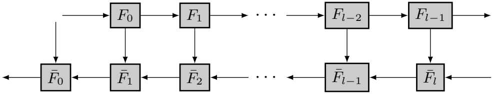


In this phase:

- We execute all F-operations;
- We write some data to disk and/or to memory.



The backward phase



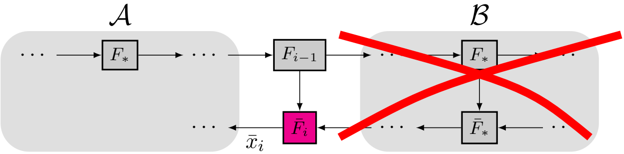
In this phase:

- We DO NOT write any data to disk (could have been done in the forward phase);
- All other operations are allowed.

No going back

Lemma

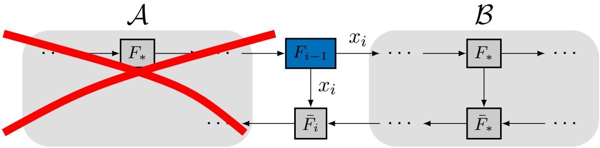
If $\bar{x}_i$ is computed, then there are no F_j for $i \leq j$ (or operations involving $\mathcal{B}$).



Checkpoint persistence (I)

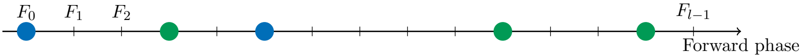
Lemma

If x_i is written (to disk or memory), until we have executed $\bar{F}_i$ there are no F_j for $j < i$ (or operations involving $\mathcal{A}$).



Checkpoint persistence (II)

In this case, for a given forward phase, we get a multi-phase backward phase:



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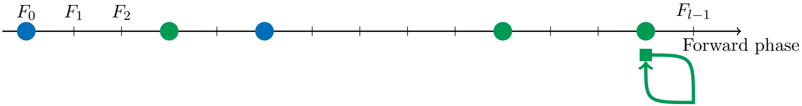

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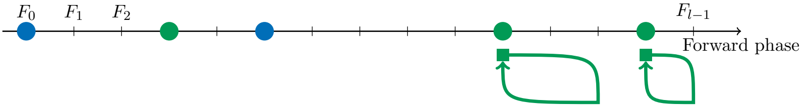

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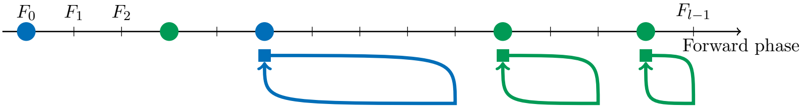

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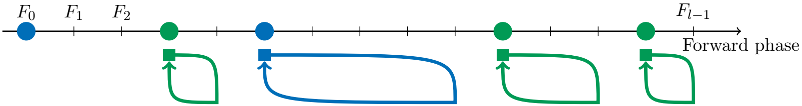

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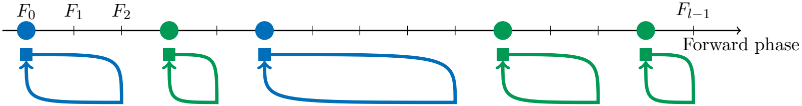
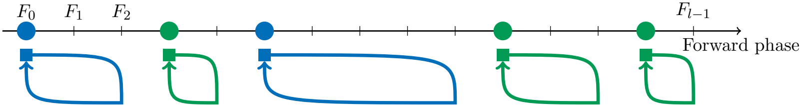


Characterizing the backward phase



- m backward steps to execute;
- No disk writes or reads;
- c memory checkpoints available

$\Longrightarrow r_m + \text{Revolve}(m, c)$

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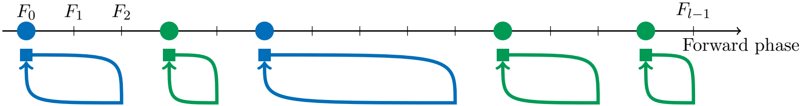

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$\Longrightarrow r_m + \text{Revolve}(m, c)$

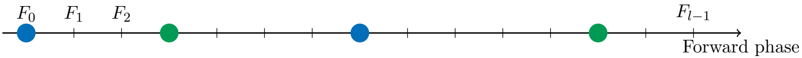
- m backward steps to execute;
- No disk writes;
- c memory checkpoints available

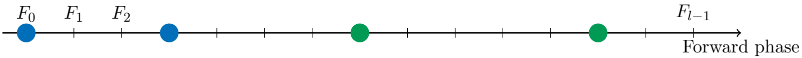
$\Longrightarrow r_d + \text{1D-Revolve}(m, c)$

Characterizing the forward phase

Theorem

During the forward phase, first we write to disks, then we write to memory.





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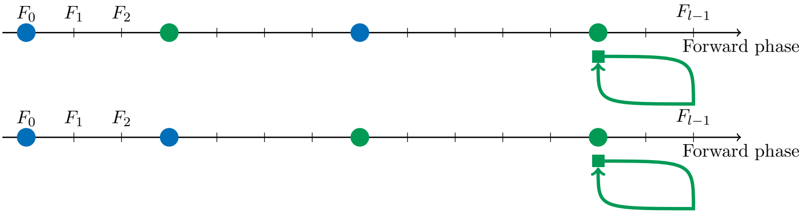

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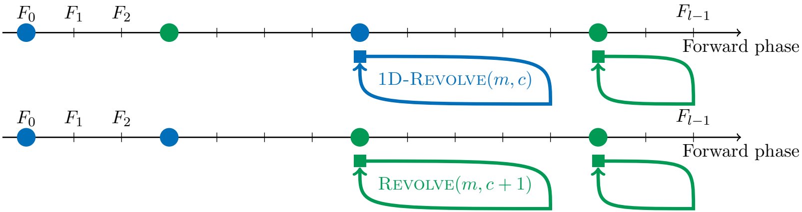

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Characterizing the forward phase

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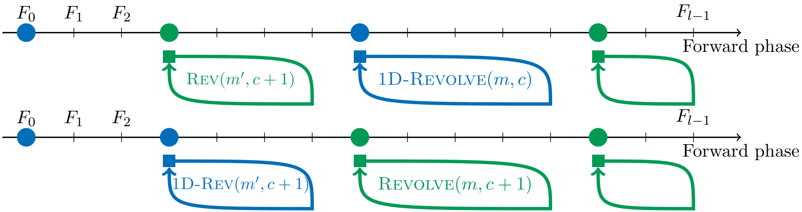

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Characterizing the forward phase

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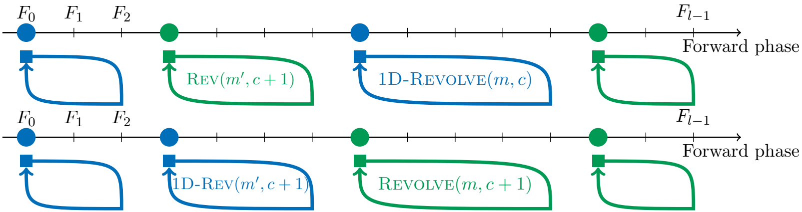

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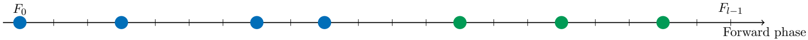
Computing the optimal schedule



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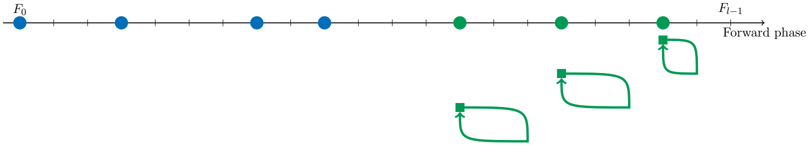

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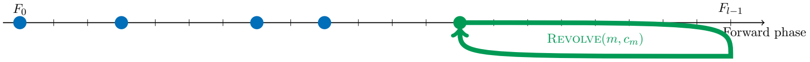

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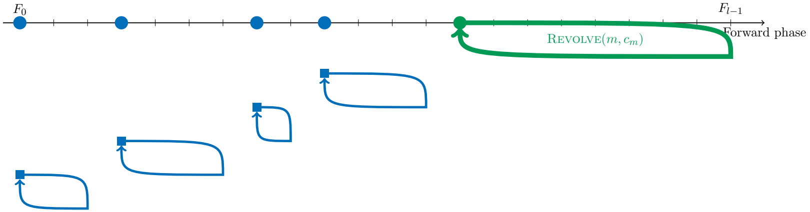

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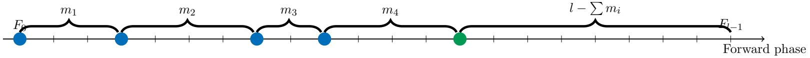

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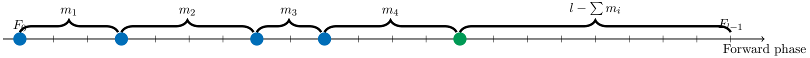
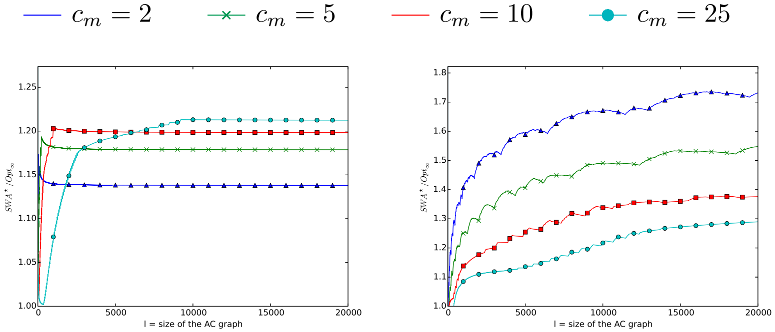


Theorem

We can compute the optimal number of disk checkpoints needed and the space between them in $O(l^2)$ with a dynamic programming algorithm to minimize execution time.

In practice?

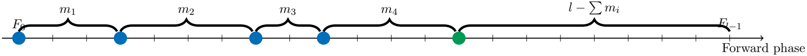
In realistic scenarios we expect to divide the execution time by 2 or 3.



(a) $w_d = r_d = 1$ (b) $w_d = r_d = 5$

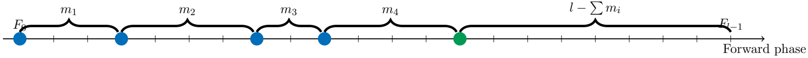
Ratio $\mathrm{SWA}^\star(l, c_m, w_d, r_d)/\mathrm{Opt}_\infty(l, c_m, w_d, r_d)$ as a function of l.

Going further



We know how to compute the m_i's. But the cost of computing them is non-negligible (l^2). Can we do better?

Going further



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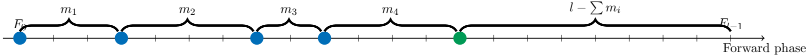
Theorem (Weak Periodicity)

Except for a bounded number of them (the bound depends on $X = (c_m, w_d, r_d)$), all the m_i's are equal (to m_X).

Going further



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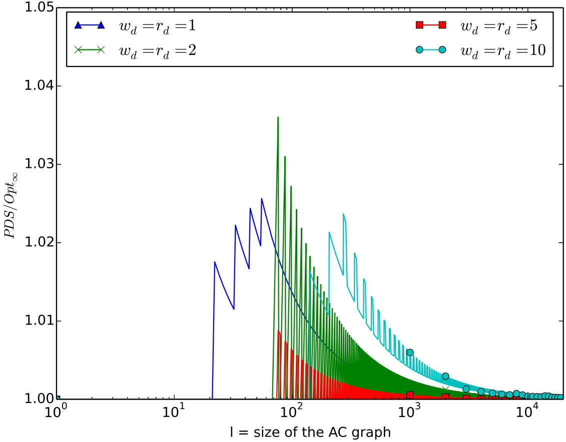
Except for a bounded number of them (the bound depends on $X = (c_m, w_d, r_d)$), all the m_i's are equal (to m_X).

Corollary

Writing disk checkpoint every m_X forward steps is asymptotically optimal.

Additional data



Makespan of periodic algo over optimal: function of l, $c_m = 10$.

Conclusions on adjoint computations

Some numbers:

- The adjoint computation in MITgcm runs in O(days), the gain induced by our optimal algorithm would be non negligible!
- Nek5000 runs on 500K cores, two processes/core on Mira. We need to take reliability into account (future work).

References:

GW00 Griewank and Walther, *Algorithm 799: Revolve: an implementation of checkpointing for the reverse or adjoint mode of computational differentiation*, TOMS, 2000

SW09 Stumm and Walther, *Multistage approaches for optimal offline checkpointing*, SISC, 2009

Perspectives on I/O management

Scalable I/O management is a critical problem for Exascale.

Some directions that need to be solved:

- Models are missing!
  Understanding applications is necessary to design better solutions.
- The energy cost of I/O management is barely studied!
  Energy is also one of the limiting factor for the next scale.
- Applications need to be redesigned!
  Some data may not be as important as other, can we find new strategies to deal with them?