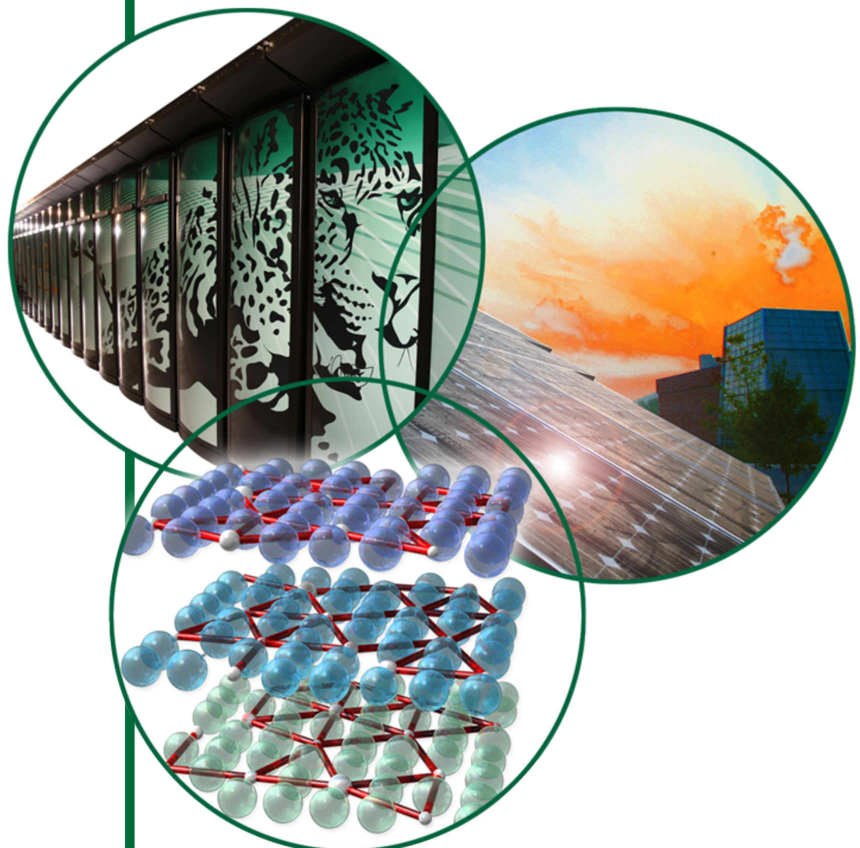
A Dependency-Driven Formulation of Parareal: Parallel-in-Time Solution of PDEs as a Many-Task Application



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U.S. DEPARTMENT OF ENERGY

SciDAC Scientific Discovery through Advanced Computing

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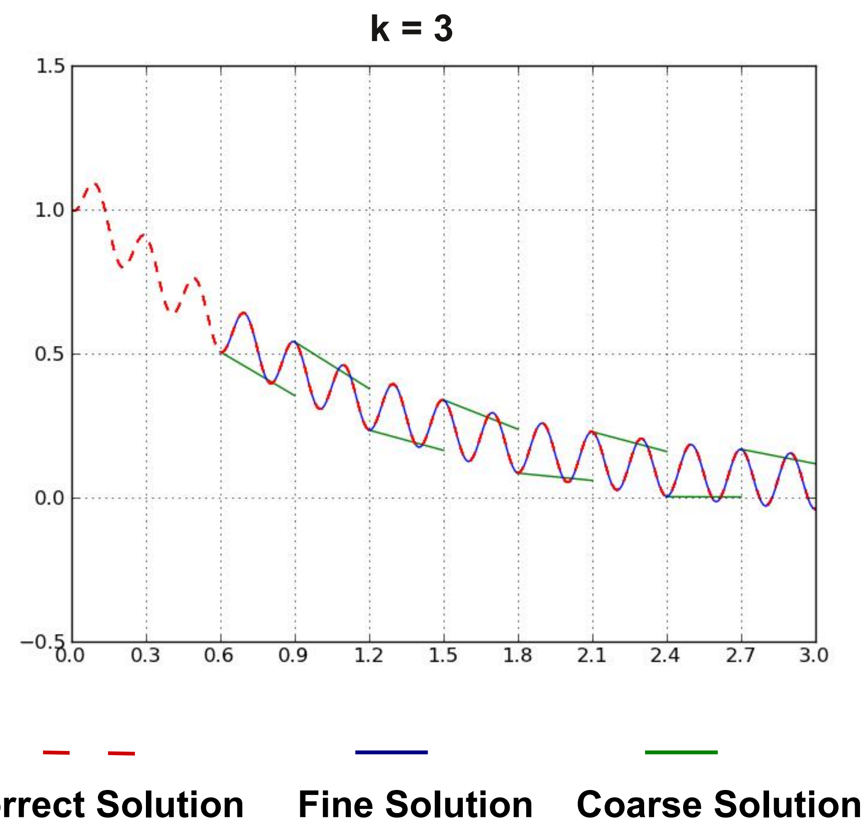
First: Shout-out to Coauthors

- **Samantha Foley, David Bernholdt, and Lee Berry**
  Oak Ridge National Laboratory
- **Debasmita Samaddar**
  ITER Organization
- **David E. Newman**
  University of Alaska, Fairbanks
- **Raul Sanchez**
  Universidad Carlos III de Madrid

Parareal: Trading Flops For Time

- Predictor-Corrector, iterative method for time-dependent PDE's
- Lions, Maday, and Turnici, 2001
- "Advance system state from initial condition λ_0 at time t_0 to time t_f, using ***N*** time "***slices***" (sub-intervals), each of size Δt, where $T = t_f - t_0 = N \Delta t$
- ***Fine,*** accurate (expensive) solver, ***F*** compute "***true***" solution
- ***Coarse***, approximate (fast) solver, ***G***, compute approximate solution
- Convergence tester, ***C***
- Guaranteed convergence in $K \leq N$ iterations
  - "Good" scenarios have $K << N$

$$F \equiv du/dt - \lambda u = sin(10\pi t)$$
$$G \equiv du/dt - \lambda u = 0 \qquad N = 10$$



Parareal: The Classic Algorithm

```
first_slice = 1
num_converged = 0
for iteration = 1, max_iterations
   for slice = first_slice..num_slices
      coarse_solve(iteration, slice)
   forall slice = first_slice..num_slices
      fine_solve(iteration, slice)
   for slice = first_slice..num_slices
      test_convergence(iteration, slice)
   num_converged +=
      first_non_converged_slice - first_slice
   if (num_converged == num_slices)
      end // SUCCESS
   else
      first_slice = first_non_converged_slice
end //Failed to converge in max_iteration
```

→ ***Sequential Phase*** (coarse_solve loop)

→ ***Parallel Phase*** (fine_solve forall loop)

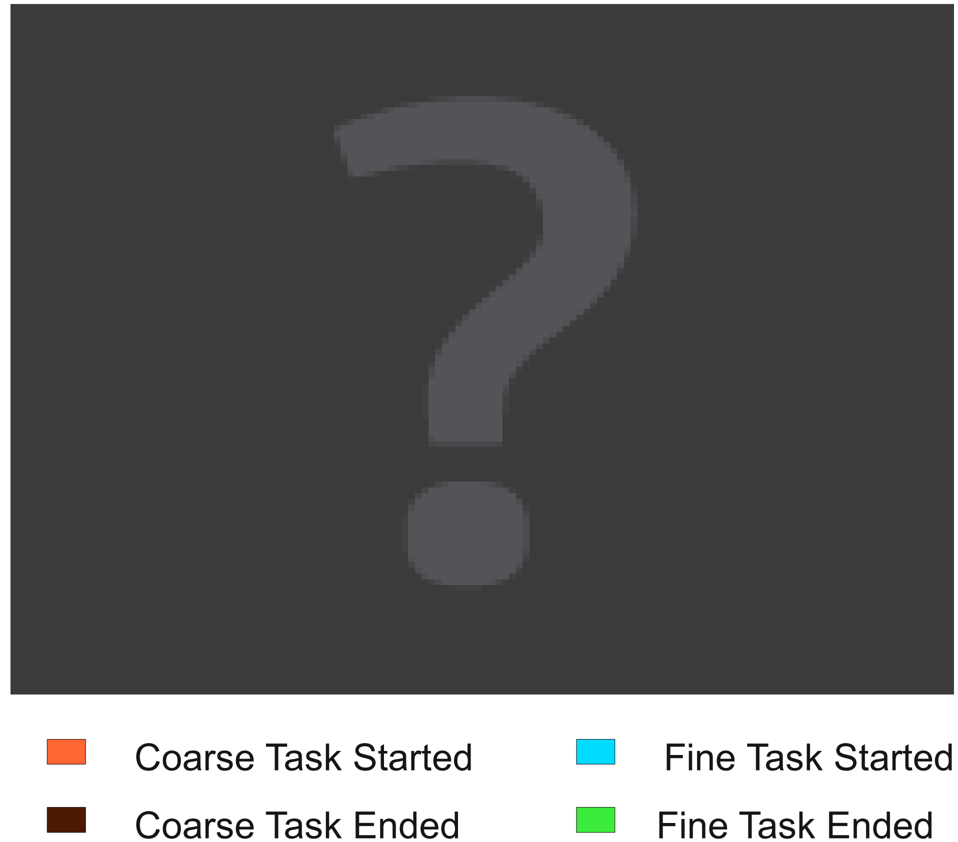
→ ***Computationally Cheap*** (test_convergence loop)

Motivational Problem

- Fusion Plasma Turbulence application (BETA) for **160** time slices on **1024** cores
- Fine solver uses **VODPK** adaptive integrator
- Coarse solver:
  - Reduced spatial resolution
  - Less accurate 4th order Runge-Kutta solver
- Implemented as a ***Many-Task*** problem
  - ***Separate MPI invocation per (coarse/fine) solve task per time slice per iteration***
  - ***File system used for inter-task data exchange***

Many Task Classic Parareal

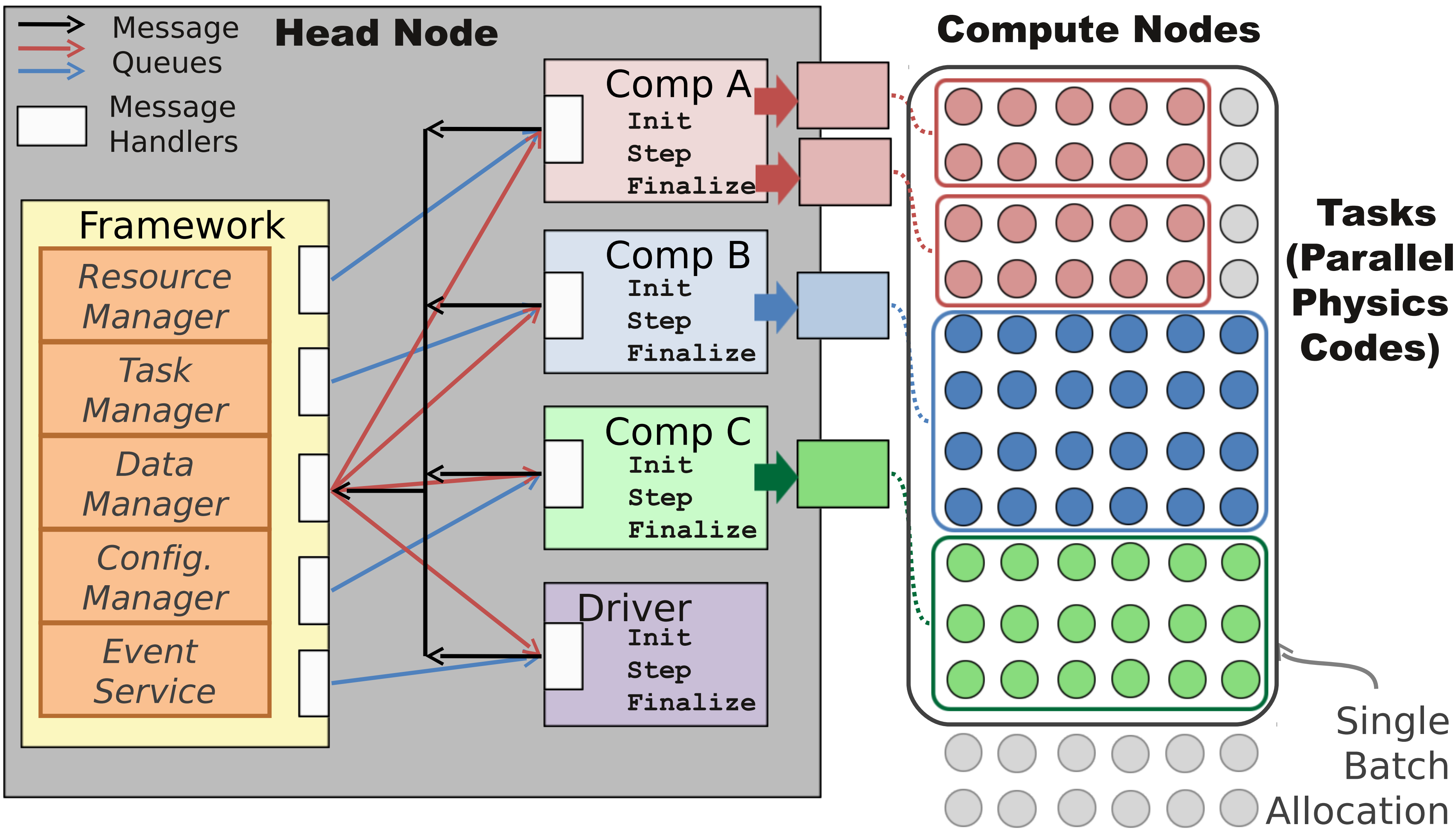
- Coarse tasks executed sequentially during each iteration
- All fine tasks for a given iteration are initiated as a single ***task pool***
  - Maximum of **64** fine solve tasks can be concurrently active on **1024** cores
- The order of task execution within a task pool is determined by the underlying execution framework
- Task Statistics:
  - Coarse Task : **16** Cores, **3.45 s**
  - Fine Task : **16** Cores, **223.15 s**
- Effective utilization: ***31.6 %***



The Underlying Framework
The Integrated Plasma Simulator (IPS)

- Component-based Python framework for loosely coupled simulations
- Originally designed for time-stepped fusion simulations
  - Flexibility allows use in other domains, and other control-flow paradigms
- Major features:
  - Thin component layer in Python that wraps stand-alone executables
  - Inter-component data exchange using the file system
  - Framework services used to assemble a simulation
    - **Resource management** - **Task management**
    - **Data management** - **Asynchronous event services**
  - Simulations execute within a single batch allocation

IPS Architecture & Execution Model



Concurrency in the IPS

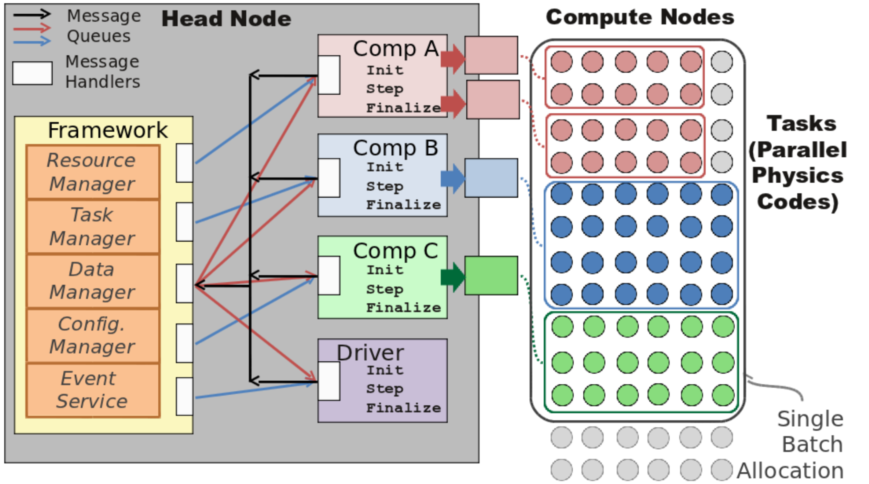
- Components launch parallel tasks
- Multiple concurrent tasks can be launched by the same component

Used to implement Classic Parareal

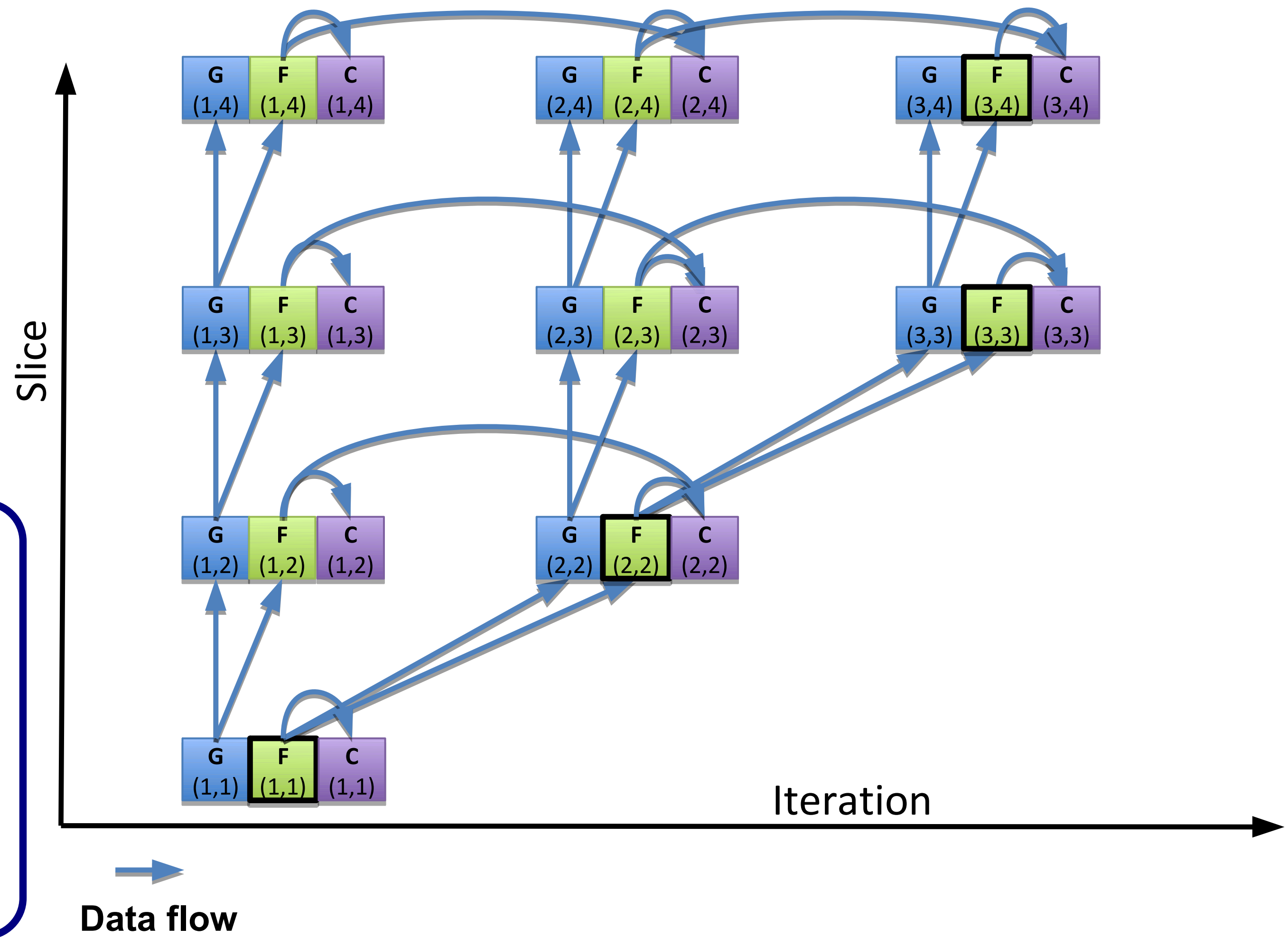
- Multiple components can be concurrently active

Used to implement Dependency-Driven Parareal

- Multiple simulations can execute within a single framework instance
  - Original IPS many-task application (see our MTAGS10 paper)



Task Dependencies in Parareal (1)

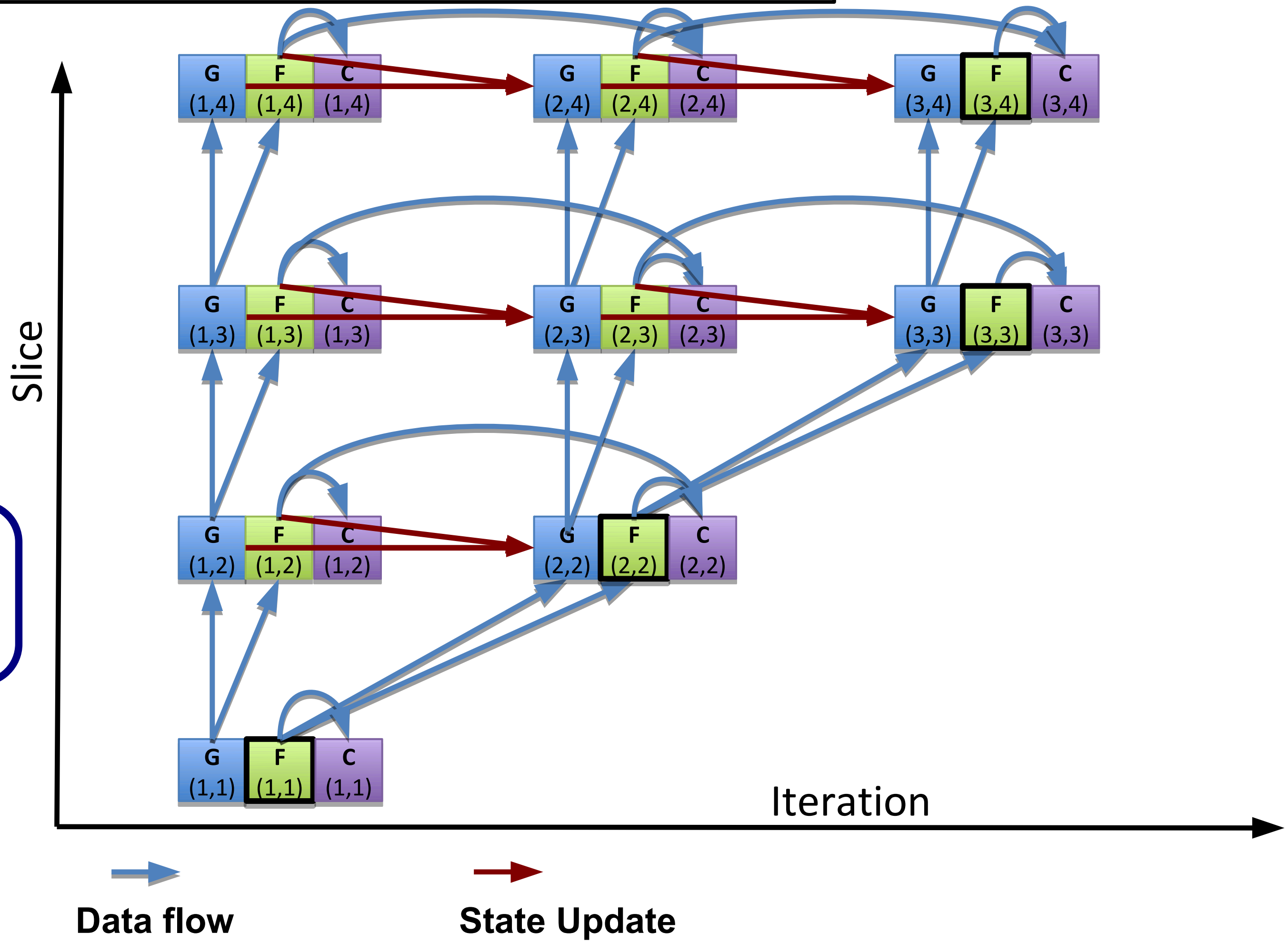


Basic ***data flow dependencies*** for computing intra-iteration coarse and fine states, and checking for convergence

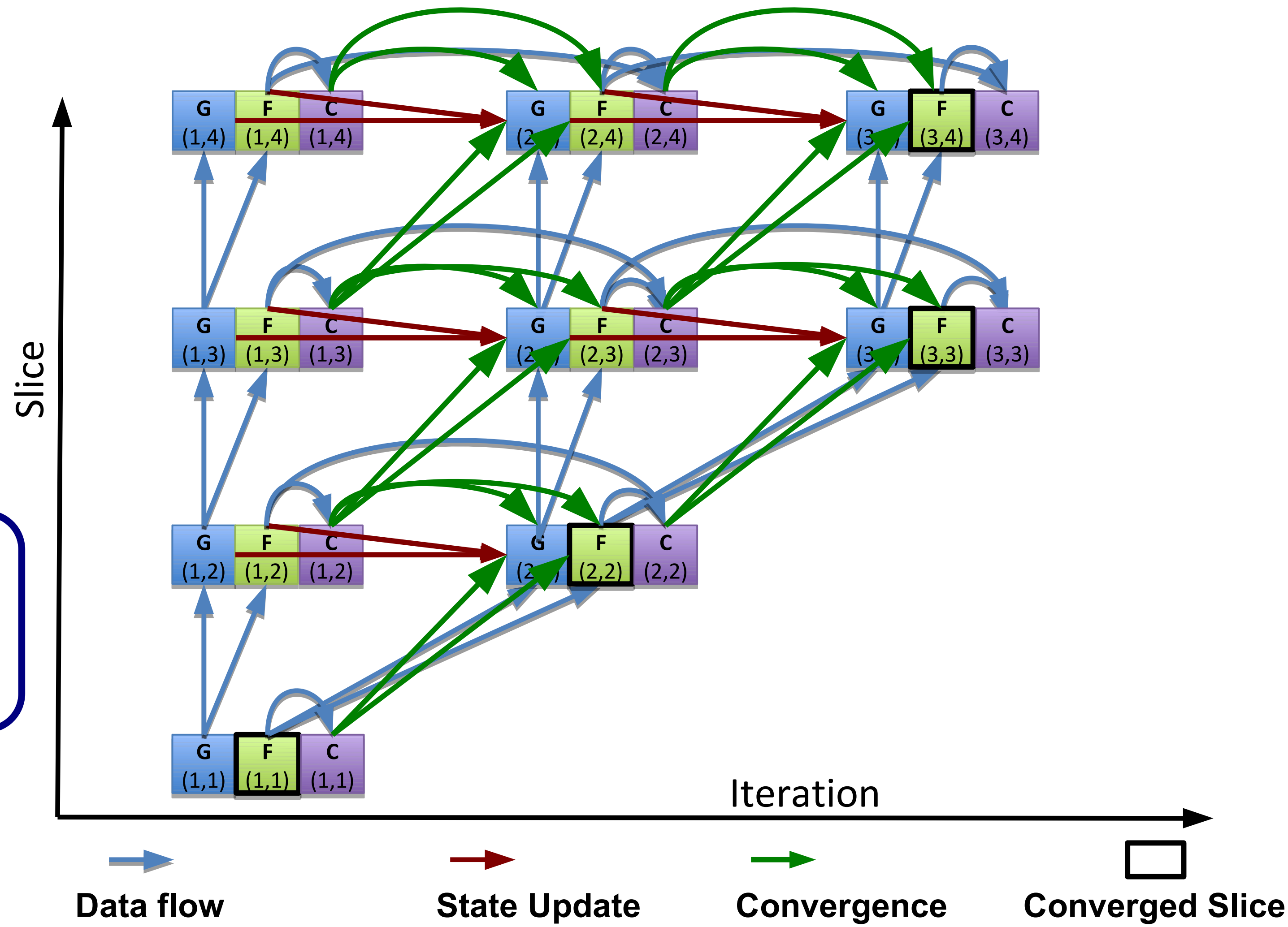
Task Dependencies in Parareal (2)

Parareal State Update $\Lambda_{k,i} = \lambda^G_{k,i} - \lambda^G_{k-1,i} + \lambda^F_{k-1,i}$

State updates "***correct***" output from coarse tasks



Task Dependencies in Parareal (3)



Convergence results control the execution of tasks in next iteration

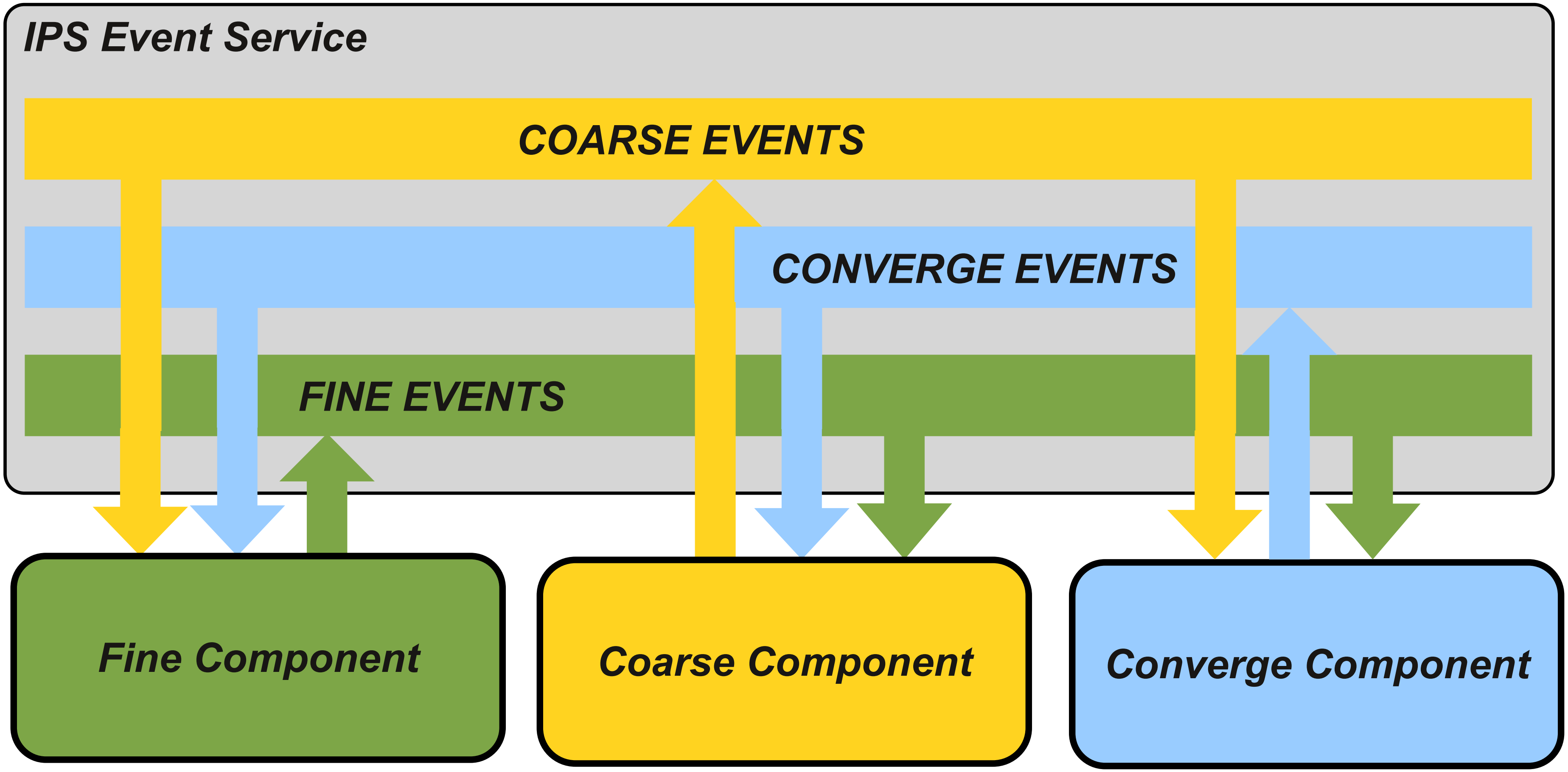
Dependency-Driven Parareal

- Three "***server***" components, **Fine**, **Coarse**, and **Converge**
- Distributed flow control:
  - Simulation logic spread across the three components
- Components initiate tasks independently
  - As as soon as ***all their dependencies are satisfied***
  - Each component encodes dependencies for its class of tasks
- Components manage their own task wait queues (FIFO)

Synchronization-reducing algorithms
- Break Fork-Join model

Jack Dongara *– Critical Issues at Peta & Exascale for Algorithm and Software Design*

Dependency Propagation Using the IPS Event Service

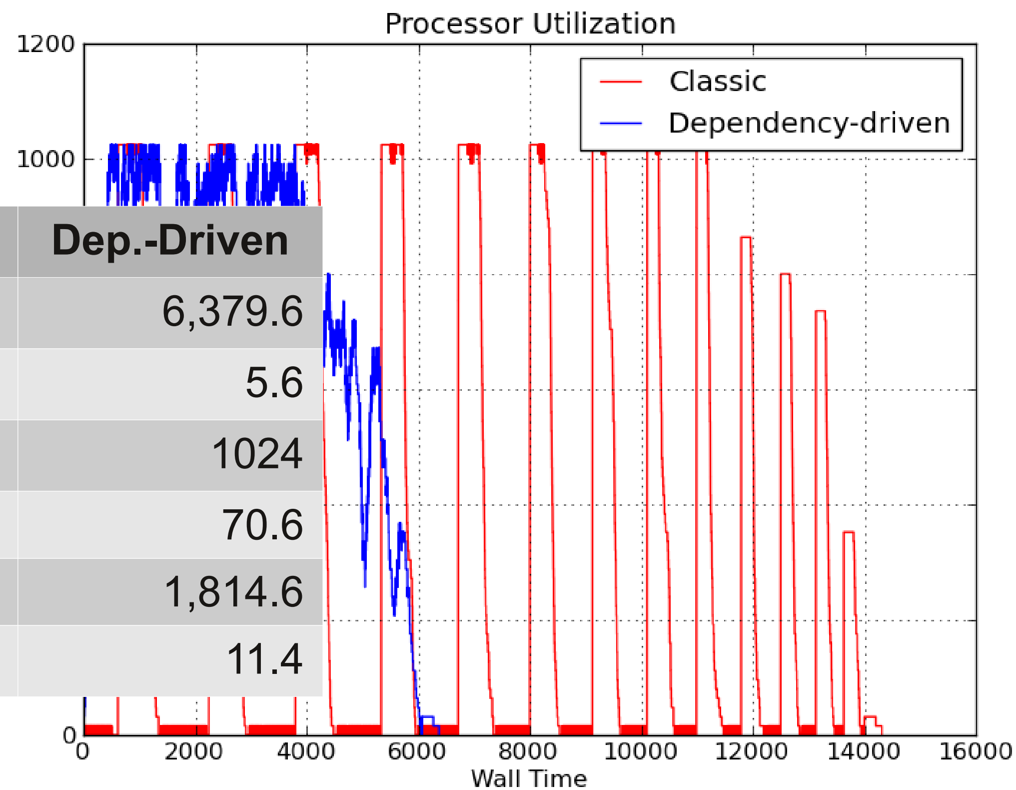


Dependency-Driven Parareal: Results

- Overlap the execution of multiple iterations
  - Up to 5 in this case
- Perform the same work done by the classic Parareal
  - Change only ***WHEN*** a task is executed
- Effective utilization: **70.6%**

Coarse Task Started
Fine Task Started
Coarse Task Ended
Fine Task Ended

Dependency-Driven Parareal: Results



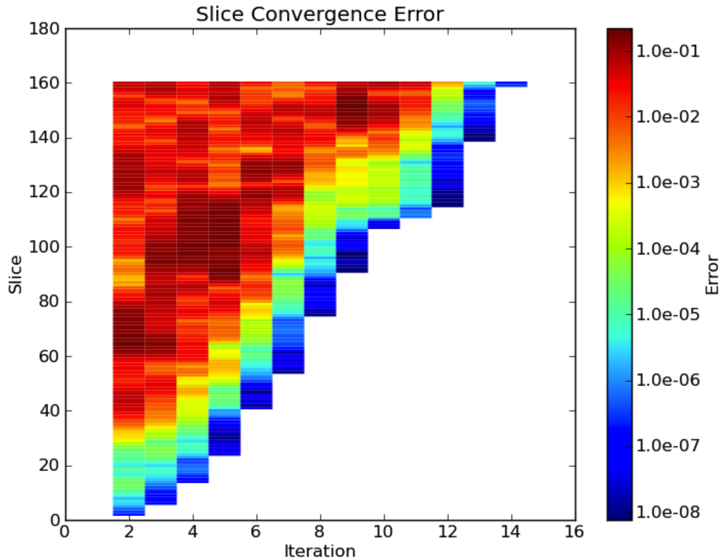
	Serial*	Classic	Dep.-Driven
Run Time (S)	35,704	14,330.8	6,379.6
Speed Up	1	2.5	5.6
Cores Used	16	1024	1024
Utilization %	100	31.6	70.6
Cost (Cpu H)	158.7	4,076.3	1,814.6
Relative Cost	1	25.7	11.4

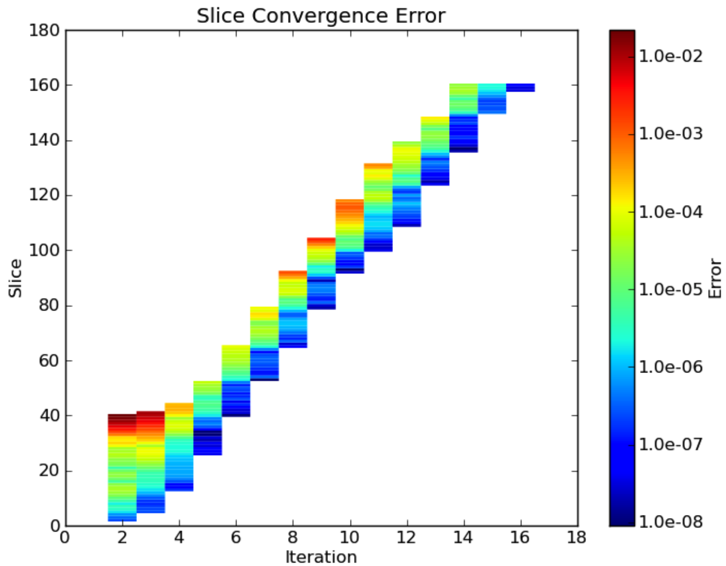
* *Estimated*

Dependency-Driven Parareal uses 44.5 % wallclock time of the classic version

Moving Window Parareal

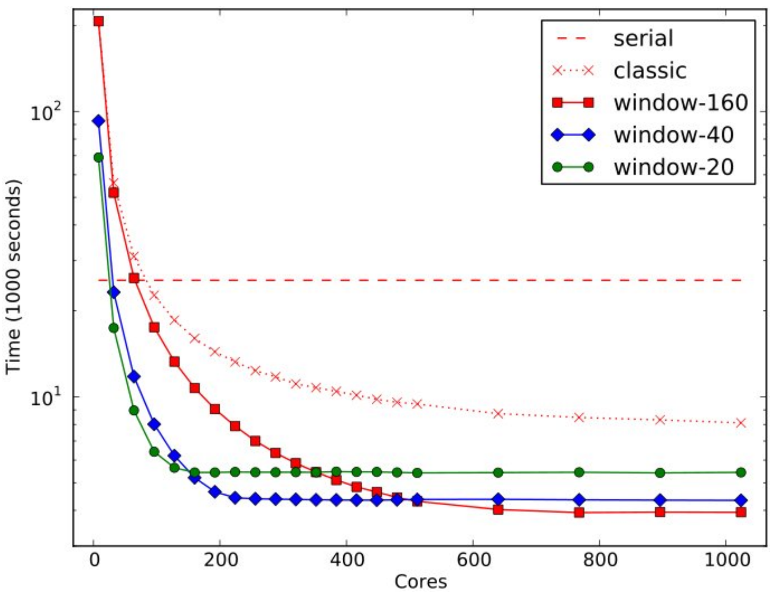
- Heat map shows convergence error per slice, per iteration (logarithmic color scale)
- Error in upper-left corner suggests limited reach of the coarse solver
  - Quality of coarse solution deteriorates as we move away from last converged result
- Optimize resource utilization by ***NOT*** executing those tasks
  - Implement a "***moving window***" version
  - Start with **n < N** slices
  - Add more, as slices converge
- Less work, less resources
  - But may need more iterations
- Introduces trade-off between window size, time to solution, and required resources



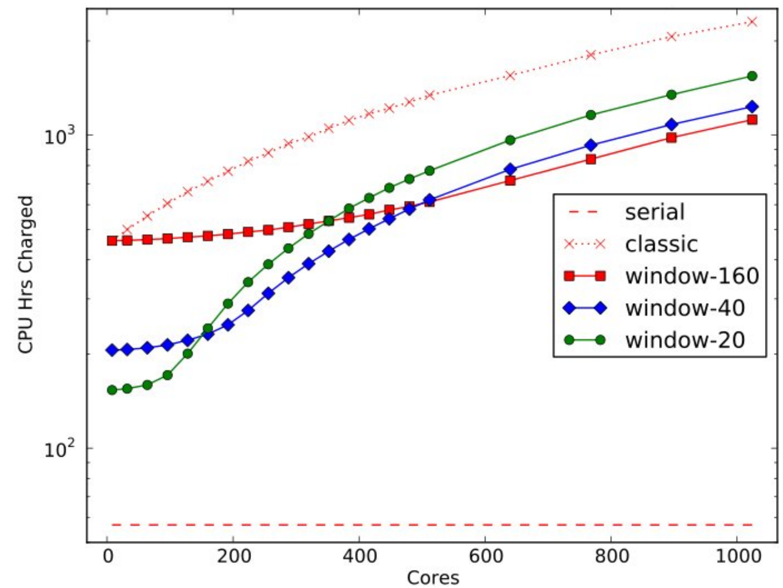


Exploring the Moving Window Parareal Trade-offs

Simulation Time



Cost



- Simulations used to explore the trade-off between resource utilization, window size, and time to solution for BETA
- Best choice depends on what's important (time, or cost ?)
- Moving window parareal allows users to choose the configuration that best meets their priorities

In Summary

- Parareal algorithm re-cast as a ***many-task problem*** executed within the IPS Framework
- ***Dependency-driven parareal*** improves resource utilization and reduces simulation time
- ***Moving window parareal*** avoids the performance of un-productive work and reduces over-all resource requirements
- Many-task implementation using IPS-parareal is:
  - Flexible – easily experiment with different coarse solvers
  - Retargettable – adapting to new problems takes less than a day's work
  - Currently being used to explore 1D MHD problems (***JOREK1D***), gyrokinetic (***GENE***) and fluid electrostatic turbulence (***TRB***)
  - Starting work on 3D MHD (***PIXIE3D***)
- *Dependency-Driven formulation should allow the use of slower (and better) coarse solvers, probably leading to faster convergence*
  - Subject of future study

Questions ?

For more info on the IPS, join us for the **PYHPC** paper

“***The Integrated Plasma Simulator: A Flexible Python Framework for Coupled Multiphysics Simulations***”,

Friday, 11:00 AM, TCC 102.

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