Integrated Plasma Simulator (IPS)

TRANSP Users Group Meeting

March 23-24, 2015
PPPL
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- **What the IPS is**
- **Example workflows implemented in IPS**
- **Possible applicability to TRANSP**
- **A miscellany of trenchant comments**

IPS? What's that? → Started under SWIM SCIDAC now part of AToM SCIDAC

The IPS is a framework that allows physics modules communicate and to efficiently interoperate

Plus a collection of physics components comprising many well known and highly tested codes

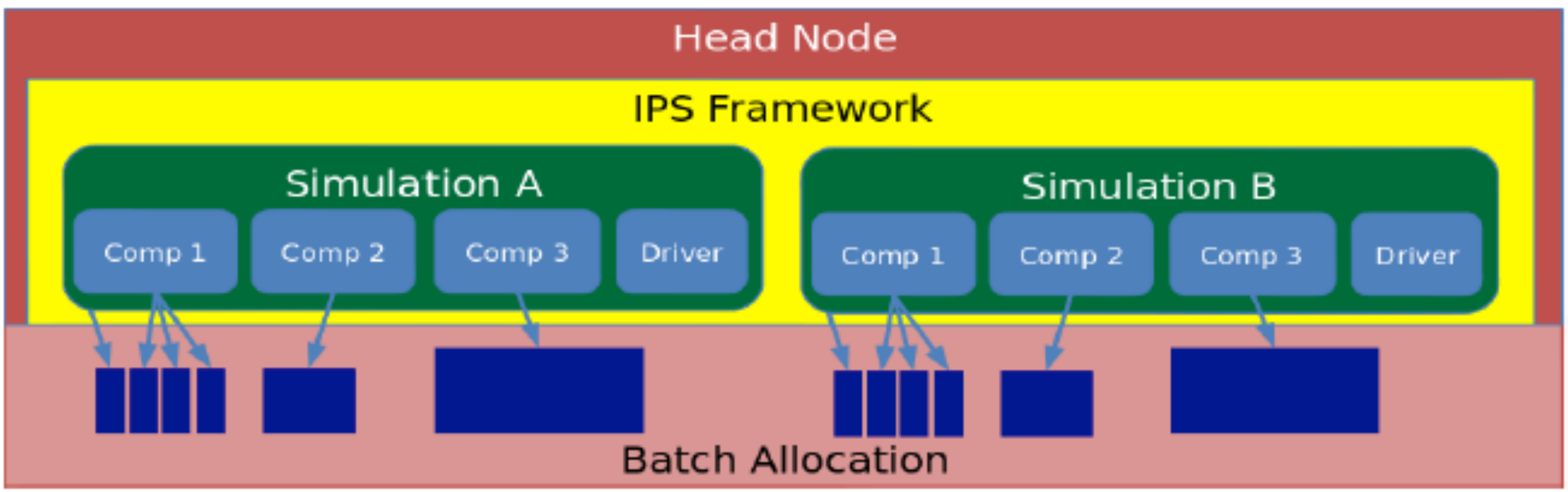
- **1.5 D transport – TSC, FASTRAN, Corsica,** ***PTSOLVER/ISOLVER in progress***
- **Neutral Beam – NUBEAM**
- **Ion cyclotron – TORIC, AORSA, GENRAY**
- **Electron cyclotron – GENRAY**
- **Lower Hybrid – GENRAY**
- **Fokker-Planck – CQL3D**
- **Gyrokinetic – GYRO, GS2,** ***TGLF***
- **Edge – EPED, SOLPS**
- **MHD – NIMROD, PEST-II …**

Design Characteristics

- **Framework/component architecture –** ***written in Python***
  - **Flexibility – multiple codes can implement components interchangeably**
  - **Extensibility – easy to add components to framework**
  - **Components can be tested stand-alone**
- **Components implemented using existing whole codes** ***(usually fortran)*** **wrapped in standard component interface** ***(written in Python)***
  - **Rapid deployment – minimize changes to physics codes to adapt**
  - **Avoid bifurcation of physics modules – no SWIM/stand-alone versions**
- **File-based communication**
  - **Zero change to physics codes – use existing I/O file structures**
  - **Avoid name-space/compiler/library incompatibilities between components**
- **Plasma State:** ***Optional*** **transfer mechanism for time-evolving data that must be transferred between components**

The IPS framework supports four levels of parallelism

- Components can launch parallel jobs – MPI code execution
- A component can launch multiple tasks concurrently – e.g. multiple flux surfaces or toroidal mode numbers
- Multiple components can run concurrently
- Multiple simulations can be managed by the framework concurrently – share resources allocated to a single batch submission (task pool)



Many code executions –> one qsub, one que wait

Capabilities of the IPS: Why you should love and use the IPS

- **Driver written in programming language (Python) – allows arbitrarily complicated component invocation → *but no python required by user***
- **Framework does the dirty work for you (provides services)**
  - Configuration management – assembles and connects needed components (config file)
  - Task management – manages execution of underlying applications
  - Data management – move/archive component input/output and plasma state files
  - Resource management – efficiently manages access to computing resources for concurrently running processes
  - Event management – provides asynchronous publish/subscribe model of data exchange in running simulation
  - Supports component Checkpoint/Restart
  - Simulation monitoring – publishes simulation meta-data and events to web-based SWIM portal
- **Monitor component aggregates time-slice data from separate physics components into viewable time series**
- **Web based portal provides real-time monitoring of simulation progress and convenient archive information on previous runs**

Web Portal Provides Snapshot of Current Status of SWIM Simulations (http://swim.gat.com:5050/)

SciDAC Scientific Discovery through Advanced Computing

swim Center for Simulation of RF Wave Interactions with Magnetohydrodynamics **Monitor**

Guest
NEW! Run Statistics | About | Login
Advanced Search
Search:

Show My Runs | Show Purged Runs [Sorted by RunID in descending order]

RunID	Rate	Purge	Status	User	Last Update	Code	Time-stamp	Wall Time	Comments
0 19162				LLUO	2011-03-29 15:04:42	Framework	3.000	1787.38	Simulation Ended
0 19161				jmrb2002	2011-03-29 14:43:43	PR-GENE11__Fine	0.000	1835.08	task_id = 9228 , Tag = 0002.0004 , Target = mpiexec --host n77,n85,n84,n82,n78,n81,n83,n80 -n 128 -npernode 16 /u1/uaf /jreynold/gene11/gene11/gene11_work/bin/pr-gene11_solver /wrkdir/jreynold/PR-GENE11.002_PARAREAL-GENE11_02_run_1_event/work/PR-GENE11__Fine_2/0002.0004 /parameters
0 19160				jmrb2002	2011-03-29 14:09:38	PR-GENE11__Coarse	0.000	647.40	task_id = 986 elapsed time = 60.86 S
0 19159				jmrb2002	2011-03-29 13:50:28	PR-GENE11__Fine	0.000	711.99	task_id = 2739 , Tag = 0002.0002 , Target = mpiexec --host n65,n64,n63,n62,n110,n111,n112,n109 -n 128 -npernode 16 /u1/uaf/jreynold/gene11/gene11/gene11_work/bin/pr-gene11_solver /wrkdir/jreynold/PR-GENE11.002_PARAREAL-GENE11_02_run_1_event/work/PR-GENE11__Fine_2/0002.0002 /parameters
0 19158				jmrb2002	2011-03-29 13:26:12	PR-GENE11__Fine	0.000	265.87	task_id = 271 , Tag = 0001.0002 , Target = mpiexec --host n114,n115,n116,n117,n110,n111,n112,n109 -n 128 -npernode 16 /u1/uaf/jreynold/gene11/gene11/gene11_work/bin/pr-gene11_solver /wrkdir/jreynold/PR-GENE11.002_PARAREAL-GENE11_02_run_1_event/work/PR-GENE11__Fine_2/0001.0002 /parameters
0 19157				Batchelor	2011-03-29 12:48:59	Framework	2.000	221.89	Simulation Execution Error
0 19156				Batchelor	2011-03-29 12:29:48	Framework	2.000	129.18	Simulation Execution Error
0 19155				Batchelor	2011-03-29 12:18:59	Framework	-1	45.60	Simulation Execution Error
0 19154				Batchelor	2011-03-29 11:16:25	Framework	101.000	380.01	Simulation Execution Error
0 19153				Batchelor	2011-03-29 11:10:04	Framework	101.000	141.23	Simulation Ended
0 19152				LLUO	2011-03-29 07:34:59	Framework	3.000	1831.65	Simulation Ended

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Each job has unique run-ID. Run data archived in MDS+. Search function allows rapid searching through the >30,000 SWIM runs stored in the system

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Many different workflows have been implemented in IPS

Conventional time loop controlled by driver component

- Transport simulations with multiple source components – ITER, Cmod, NSTX

Time loop controlled by one of the components

- NIMROD with GENRAY to study ECCD stabilization of tearimg modes

Iteration loop, rather than time loop

- FASTRAN with TGLF transport and source components iterating to self consistency

Concurrent execution within component

- Full ICRF antennal toroidal mode spectrum concurrent with TORIC

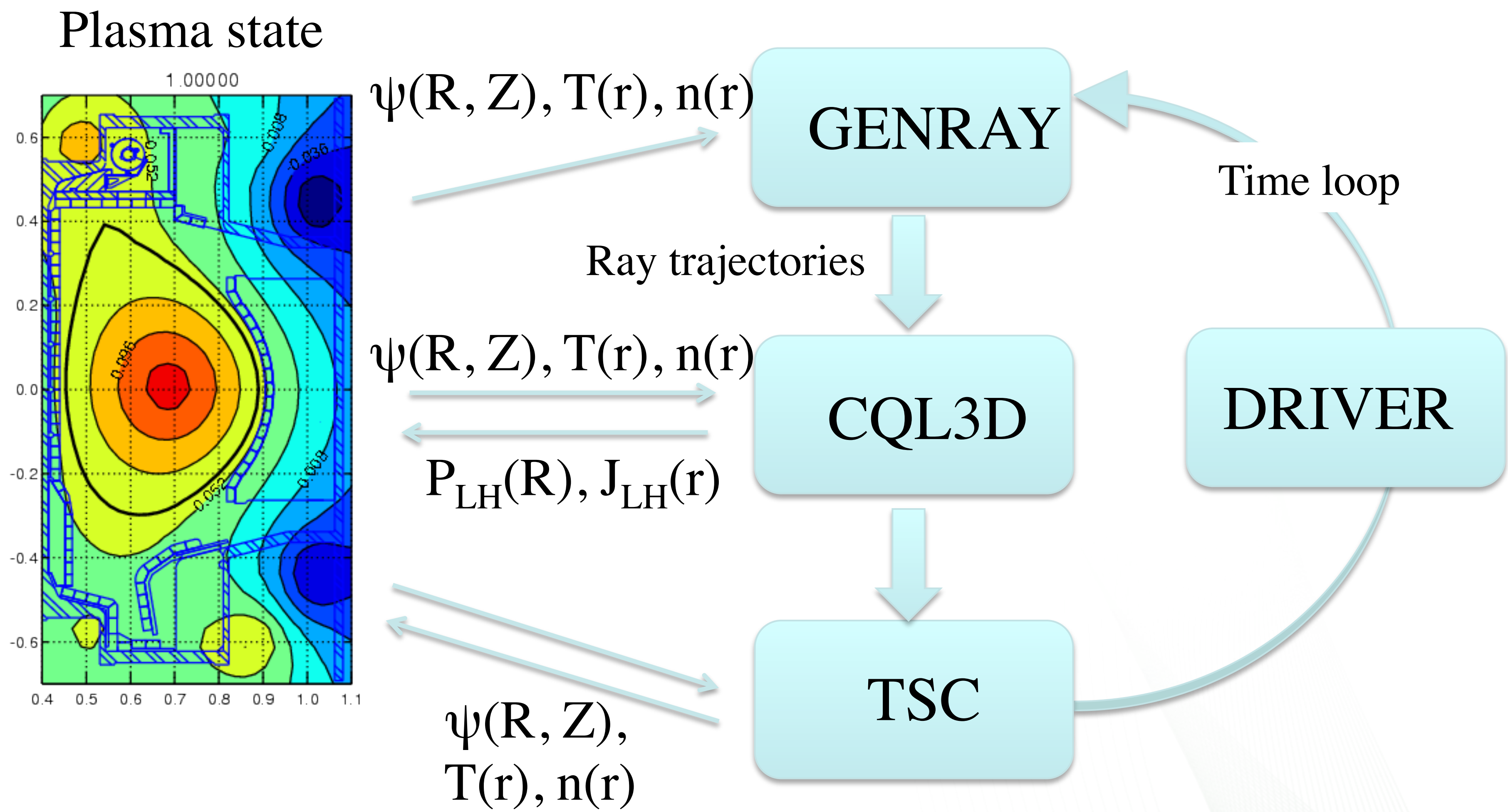
Parareal – hybrid time/iteration loop with logic embedded in components.

- An iterative algorithm for parallelization over time
- Time domain divided into chunks, iterative correction of time chunks run concurrently
- Multiple time chunks at different iteration levels running concurrently

IPS coupled with DAKOTA – optimization searches and parameter sweeps

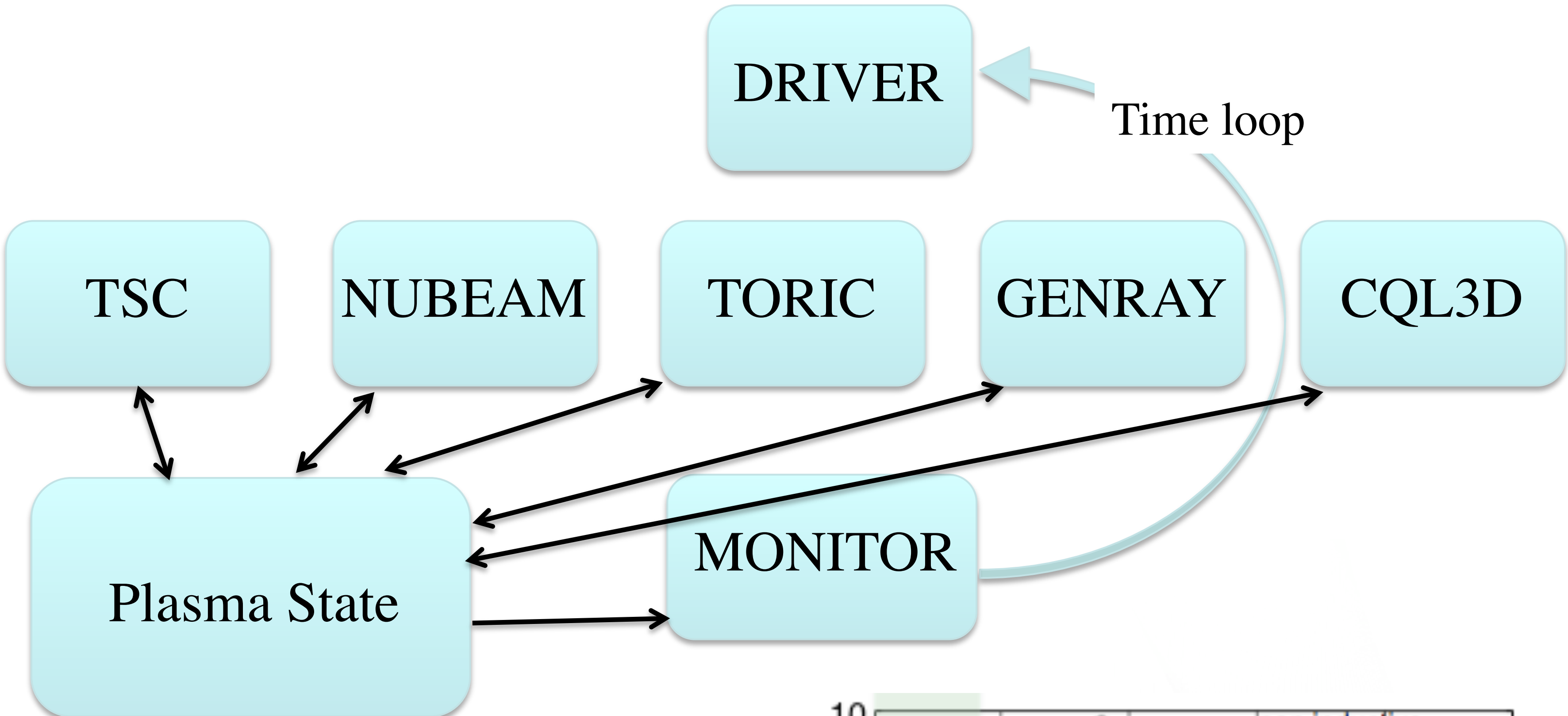
- Manages large numbers of essentially serial jobs

Simple, explicit time loop coupling lower hybrid RF (GENRAY), Fokker-Planck CD (CQL3D), and transport (TSC)

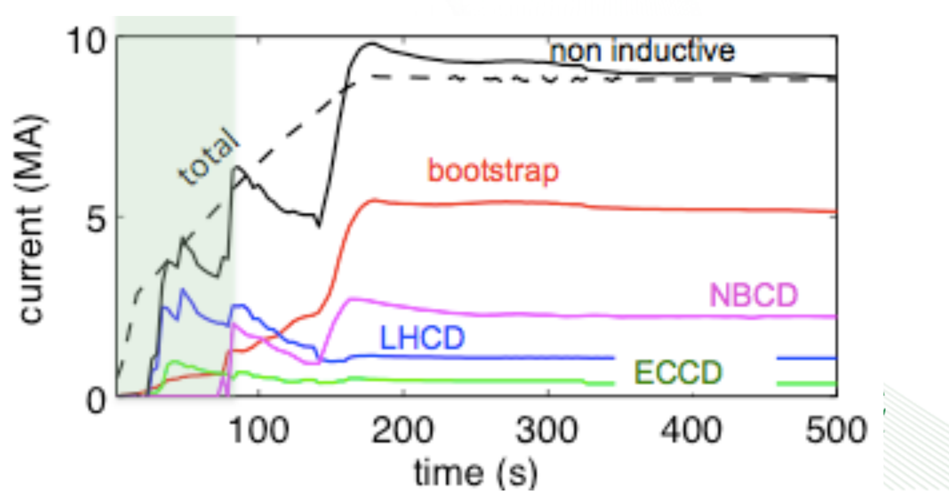


Application: Time-domain simulation of nearly fully non-inductive discharge in C-Mod using LHCD (Bonoli *et al*)

Explicit time stepping with concurrently running components

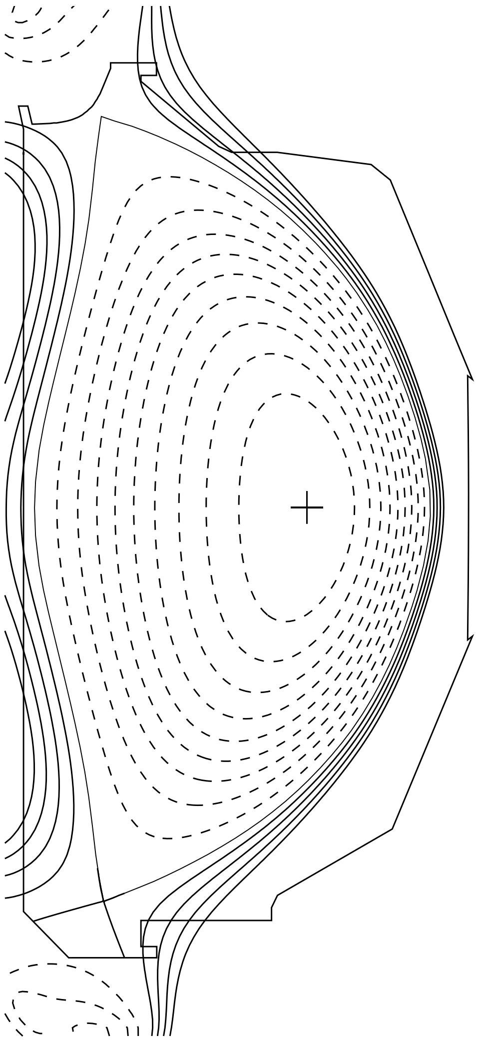


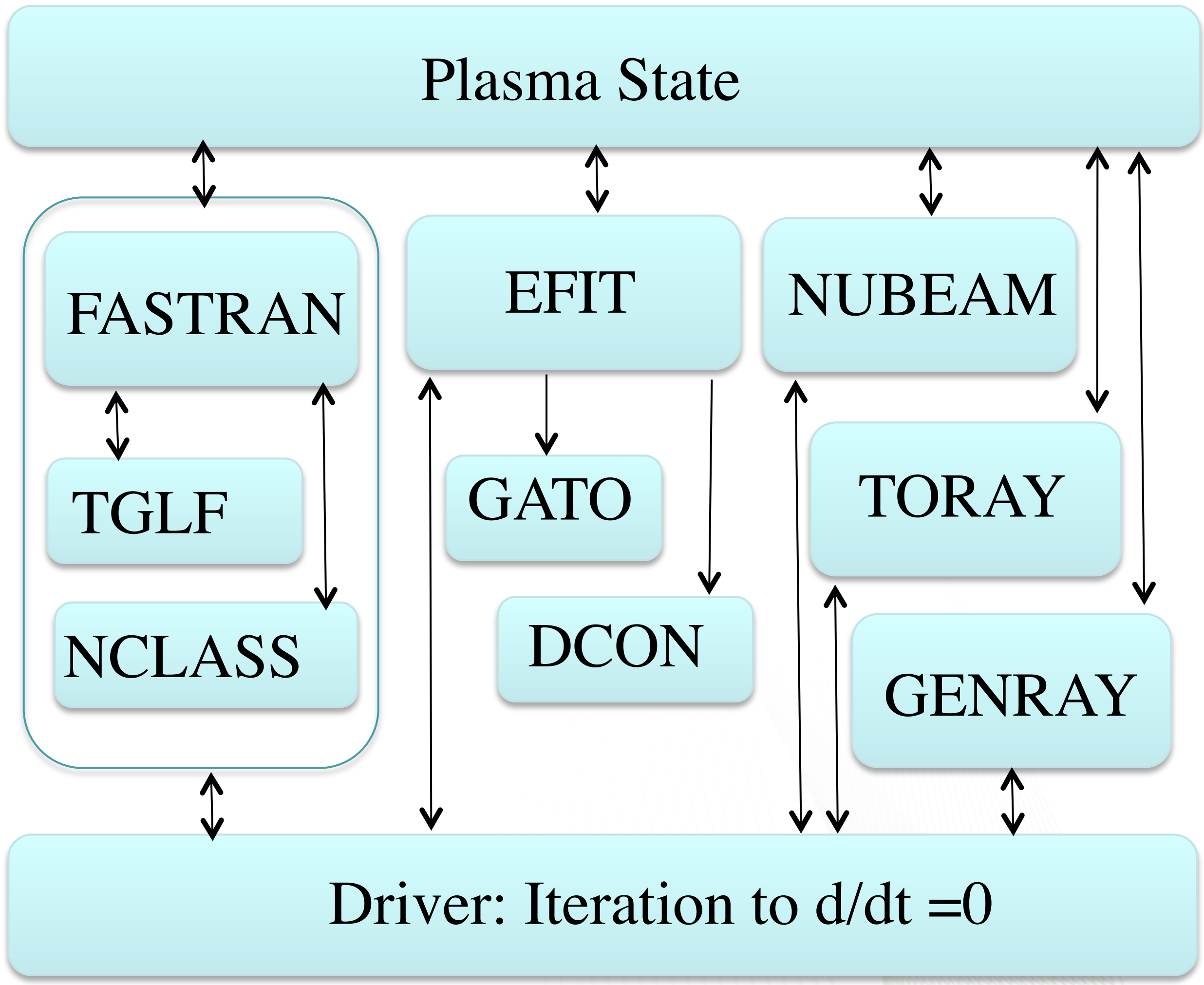
Application: ITER scenario studies (Poli *et al*)



Fixed-point iteration: FASTRAN with TGLF transport and source components iterating to self-consistency

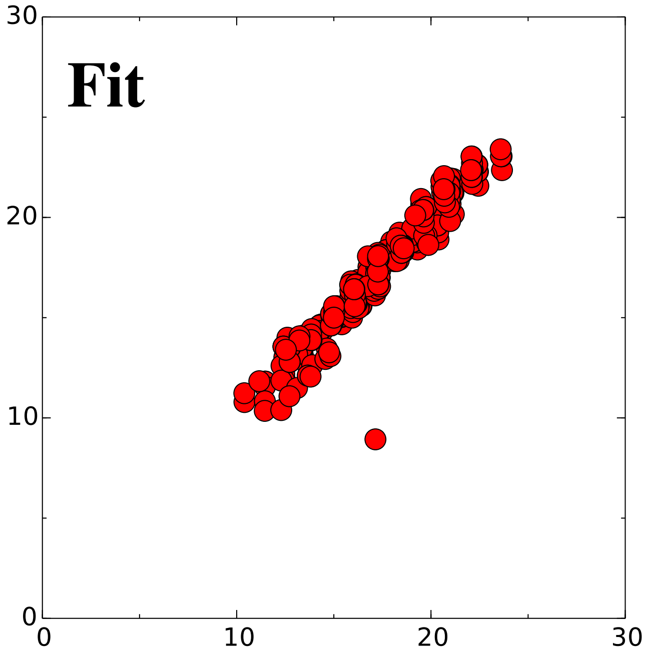
Self-consistent DIII-D equilibrium at $\beta_N = 5$



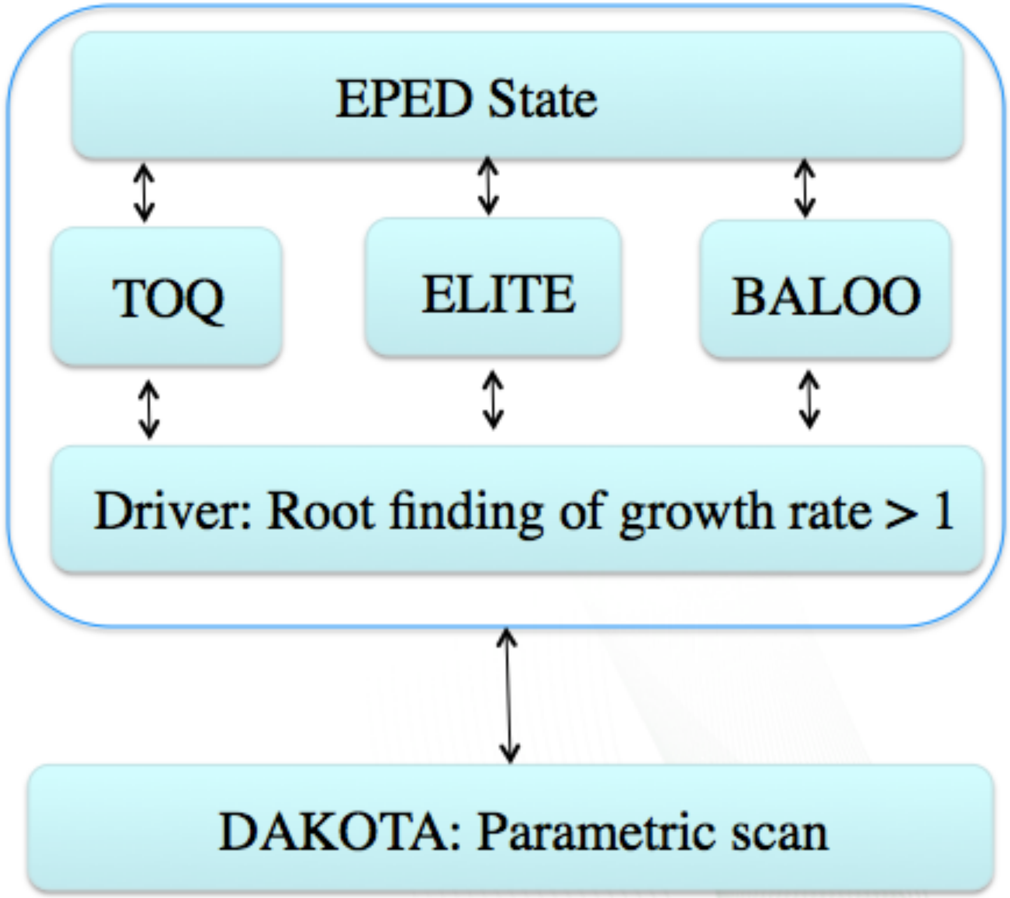


DAKOTA-Enabled IPS – EPED scans and GYRO scans

Regression for 500 EPED runs for DIII-D SS scenario

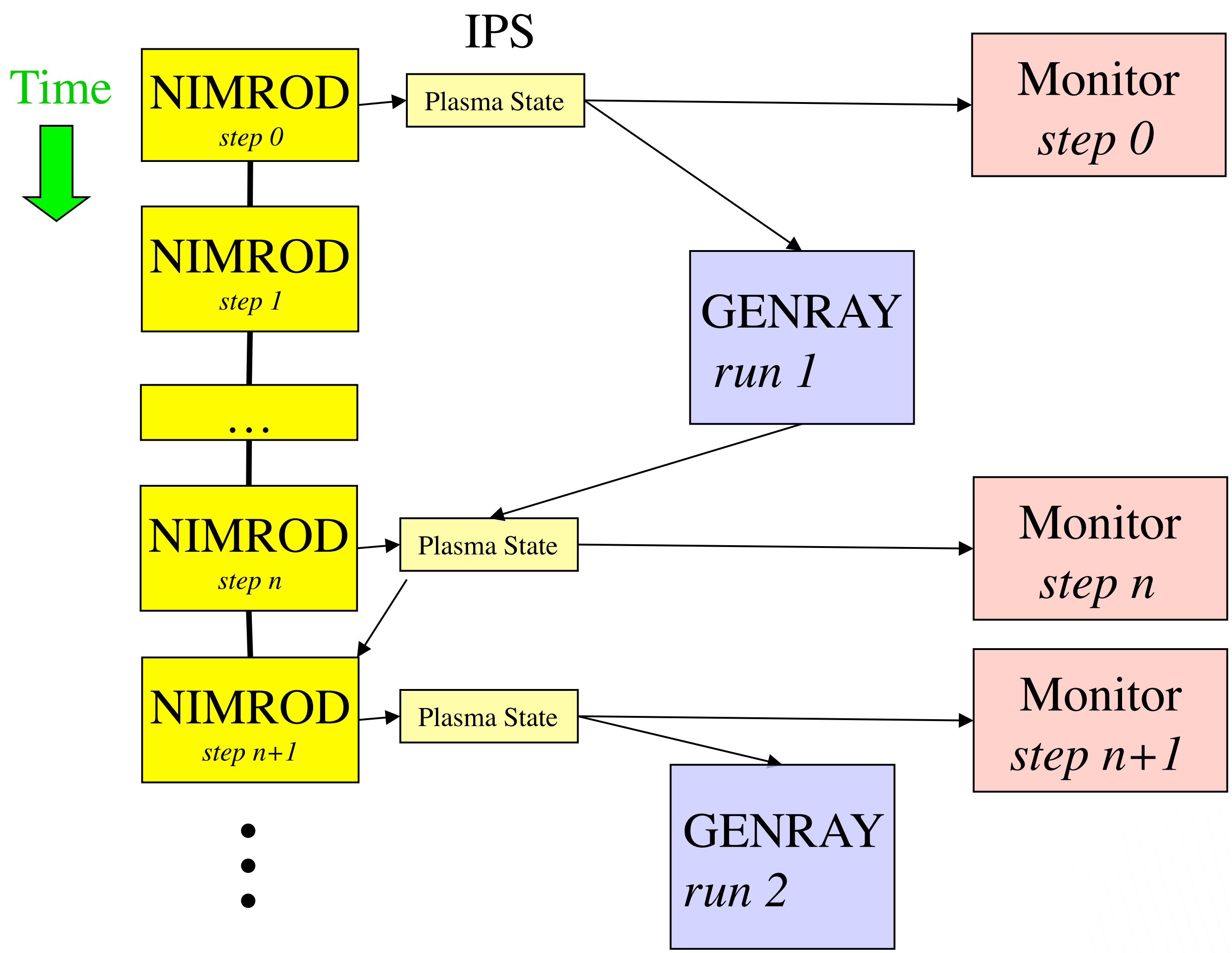


P_{ped} (kP), EPED



Application:
Parametric fit to EPED database (Park *et al*)
Recalibration of TGLF – GYRO (Candy *et al*)

NIMROD/GENRAY coupling in IPS – NIMROD is run as a service, but controls time loop via simulation *event handling*

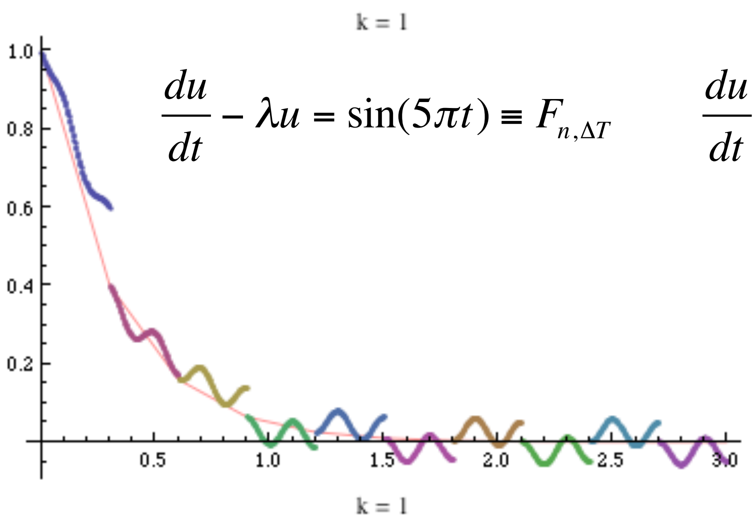


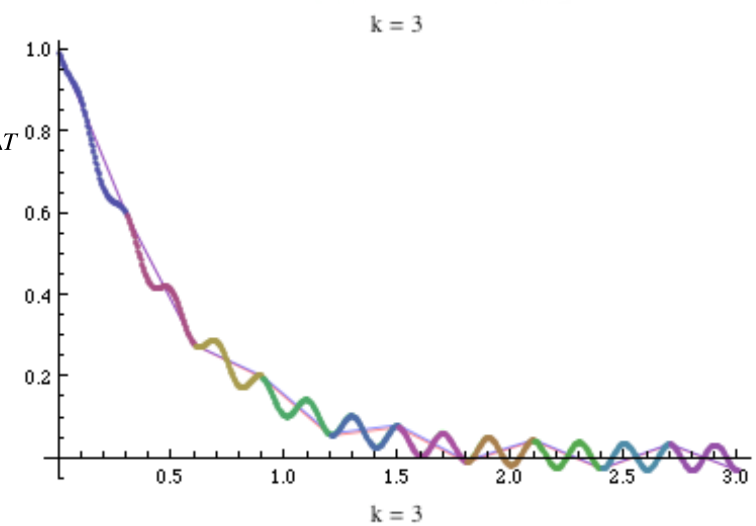
- **NIMROD exports magnetic geometry and n,T profiles to Plasma State**
- **GENRAY then calculates RF propagation and power deposition; exporting these quantities to the Plasma State**
- **NIMROD converts GENRAY data into momentum and energy source terms.**
- **Ultimately will include kinetic closure model**

Completely event driven workflow – Parallelization over time domain using parareal algorithm

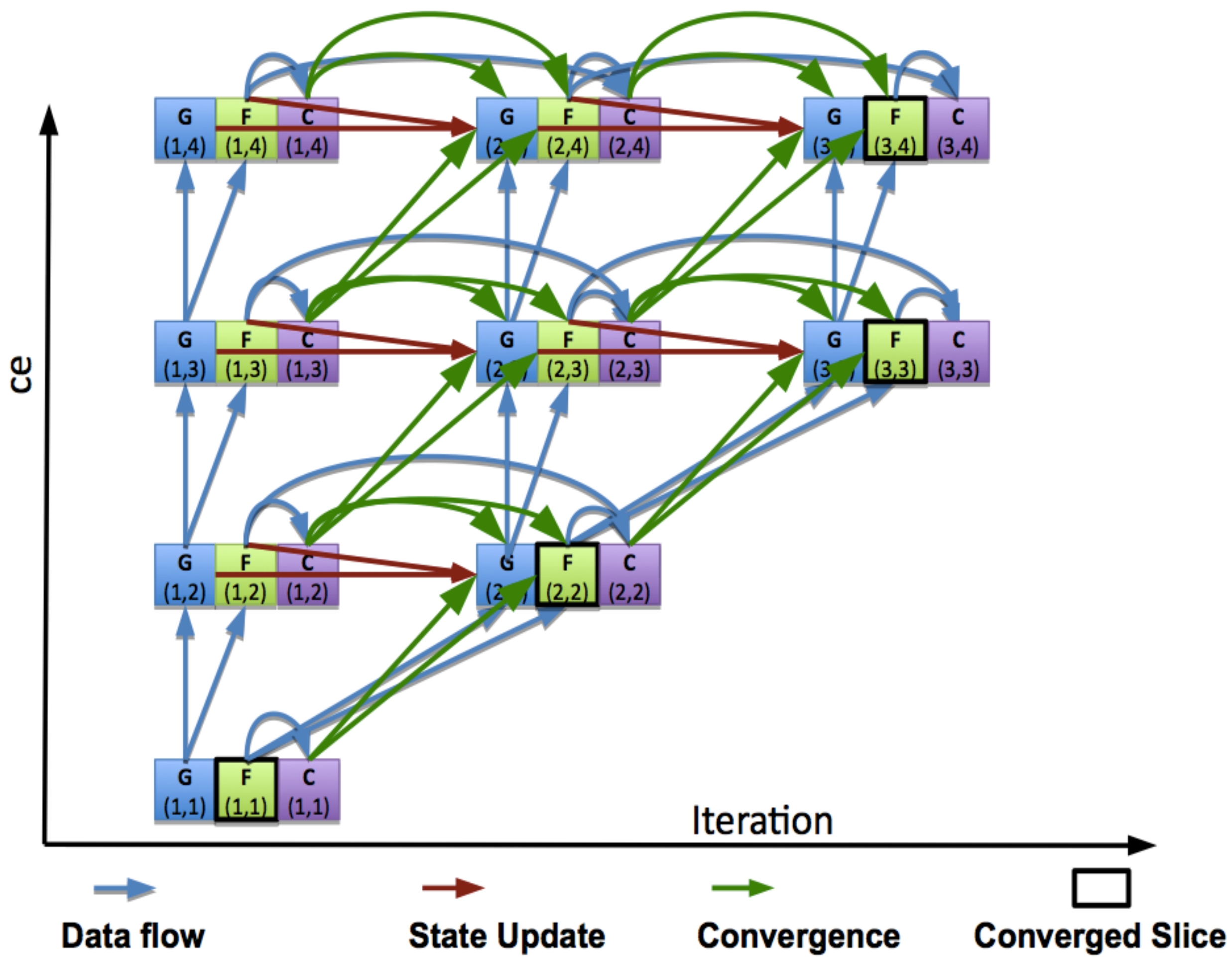
- **Requires :**
  - **Accurate solver, *F(x, t)*, you want to solve from t_{init} to t_{final} → *fine solver***
  - **Fast, less accurate solver, *G(x, t)* → *coarse solver***
  - **Convergence criterion for solution x**
- **Break time domain into a large number of chunks, NΔT**
- **Run coarse solver get approximate solution**
- **Run fine solver in parallel using coarse solution as starting point for each time chunk**
- **Parareal algorithm – iteration scheme connecting coarse and fine solutions guaranteed convergence in N interations, but maybe much faster**

$$\frac{du}{dt} - \lambda u = \sin(5\pi t) \equiv F_{n,\Delta T} \qquad \frac{du}{dt} - \lambda u = 0 \equiv G_{n,\Delta T}$$





Logic contained in components (not driver) – event driven based on availibility of data



Applications:

- **DTEM turbulence – BETA**
- **1.5D transport – Corsica**
- **Edge – SOLPS**
- **Gyrokinetics – GS2**

Samaddar *et al*

Good when time is expensive and processors are cheap

What is IPS good for?

- **Implementing complex workflows – on any scale computer**
- **Coupling massively parallel codes, or codes with varying degrees of parallelism**
  - **Can greatly increase throughput using multi-level parallelism**
  - **Particularly useful if we already have the physics components you need**
- **Managing large numbers of related serial or parallel jobs**
  - **Parameter sweeps**
  - **Optimizations**
- **We have in hand a number of useful workflows you can take *gratis***

SWIM aimed to make it easy (at least possible) to add new components, interchange components, generate workflows, use compute resources efficiently

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How do you use IPS? What do you get?

- **User provides a configuration file to specify simulation elements + input files for the component codes**
- **Submit from the command line (e.g. qsub) – *or now through OMFIT***
- **Output is a "results" directory tree consisting of selected physics code output files + Plasma State files (if using)**
- **Also get monitor component – aggregation of selected state data into time-series**
- **Web-based monitoring of job progress. Ability to view monitored data as job runs**

AToM project aims to make it easier for users to set up and analyze IPS runs through coupling to OMFIT

Initial thoughts on application to TRANSP

- **We think that it should not be difficult for TRANSP and IPS to interact – they both speak Plasma State**
- **TRANSP could actually be incorporated as an IPS component**
  - **Could make massively parallel computing more accessible to TRANSP users**
  - **User-efficient/resource-efficient way to do multiple related TRANSP runs or very long runs**
- **TRANSP could spin off IPS sub-workflows**
  - **e.g. have IPS run all RF/Neutral Beam components concurrently**
  - **Implement complicated workflows not already contained in TRANSP**
- **Interpretive mode**
  - **TRANSP generates time sequence of experimental plasma profiles → Plasma States**
  - **IPS runs all source modules concurrently on all time slices, returns plasma states with heating/CD profiles**
- **If it is decided to refactor TRANSP into a more modular structure, IPS might be considered for the framework**

Other thoughts and questions

- **Plasma State**
  - We consider it to be a valuable resource
  - What is PPPL plan on future development/support?
- **Interacton with ITER**
  - We need experience with IMAS and ITER data structures
  - PPPL do Plasma State to IMAS translation
  - Plan to install IMAS at PPPL – schedule and details?
  - We will want to keep US-based simulation capability for our own purposes
- **AToM now working on nested IPS simulations**
- **There are significant advantages to discrete code architecture vs single executable**