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Design Elements of EFFIS and Weak & Strong Couplings in CPES

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Center for Plasma Edge Simulation

Design principles demanded by CPES codes: EFFIS should

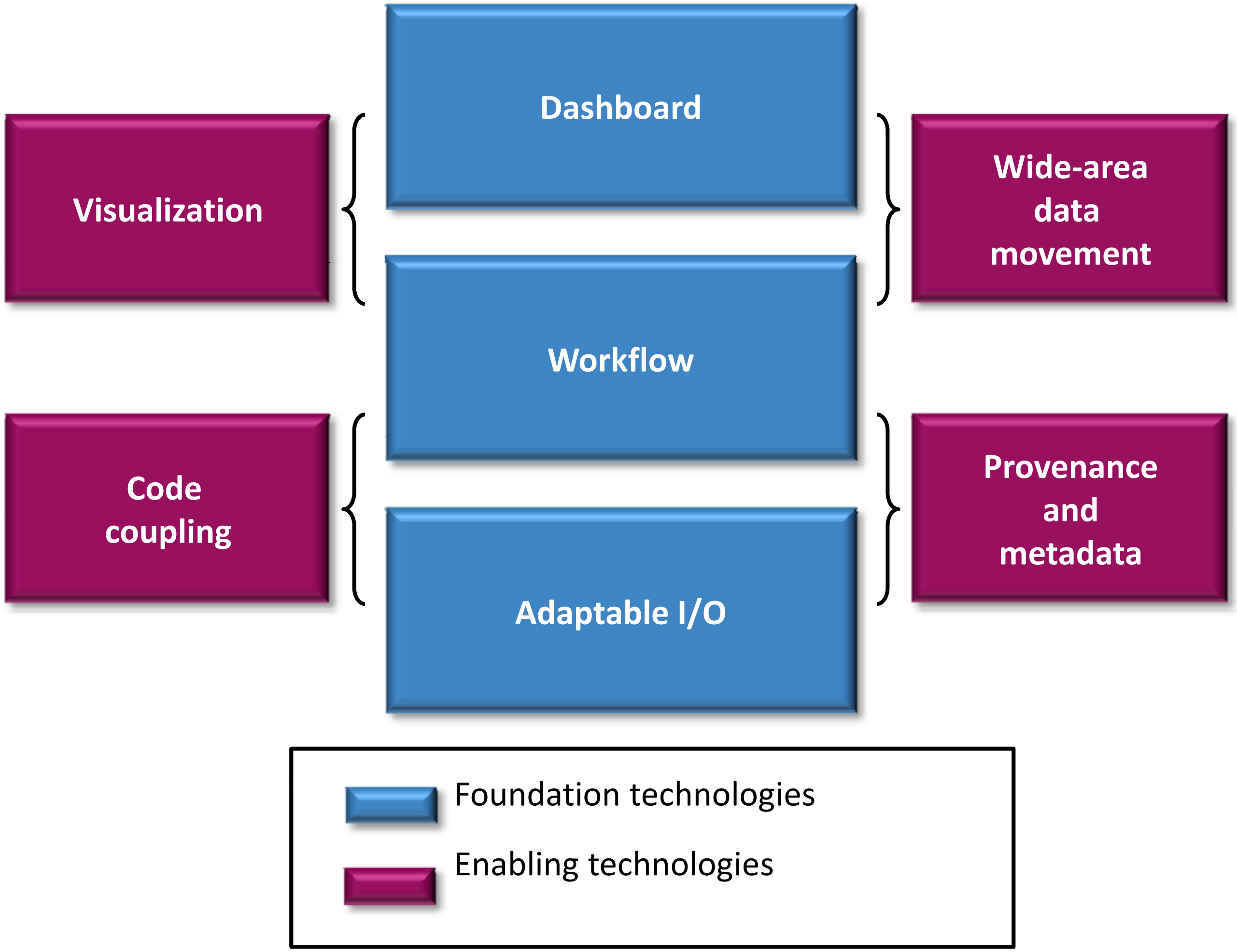
- Accept widely-different physics codes without discrimination
  - ✓Single processor to extreme scale parallelism
  - ✓PDE and Monte Carlo
  - ✓In-memory and file-based together
- Allow the unit codes to keep their independence
  - ✓To be "**living**" science services by allowing continuous development and transformation of unit codes into the future
  - ✓To allow each unit codes to use their own compilers and options, and library version

  → Coupling through I/O layer only with simple APIs
- Have long lifecycle
- Include automated workflow with real time monitoring and analysis capabilities and provenance capturing
  - ✓Supported by efficient and reliable **data mover**
- Have "living" **framework tools** to serve
  - ✓Continuously evolving science drivers and
  - ✓Rapidly changing hardware/software environment

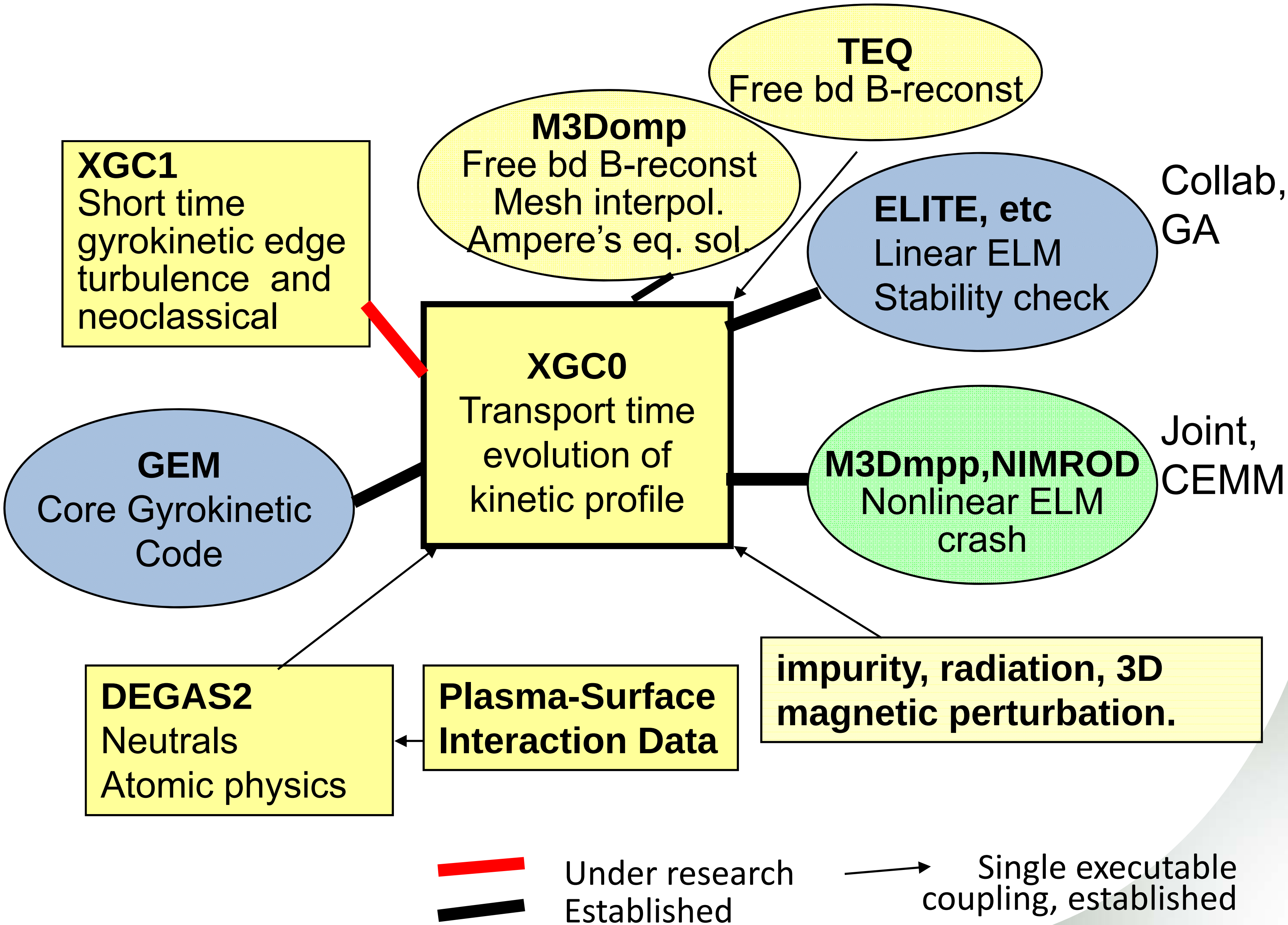
→ **EFFIS with Service Oriented Architecture**

CPES uses modern computer science tools

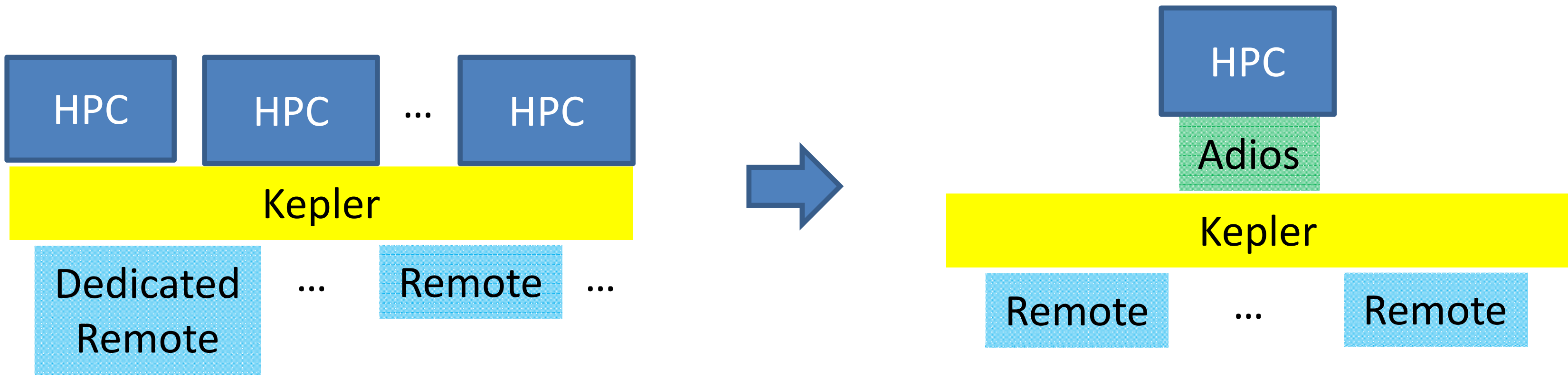
EFFIS tools



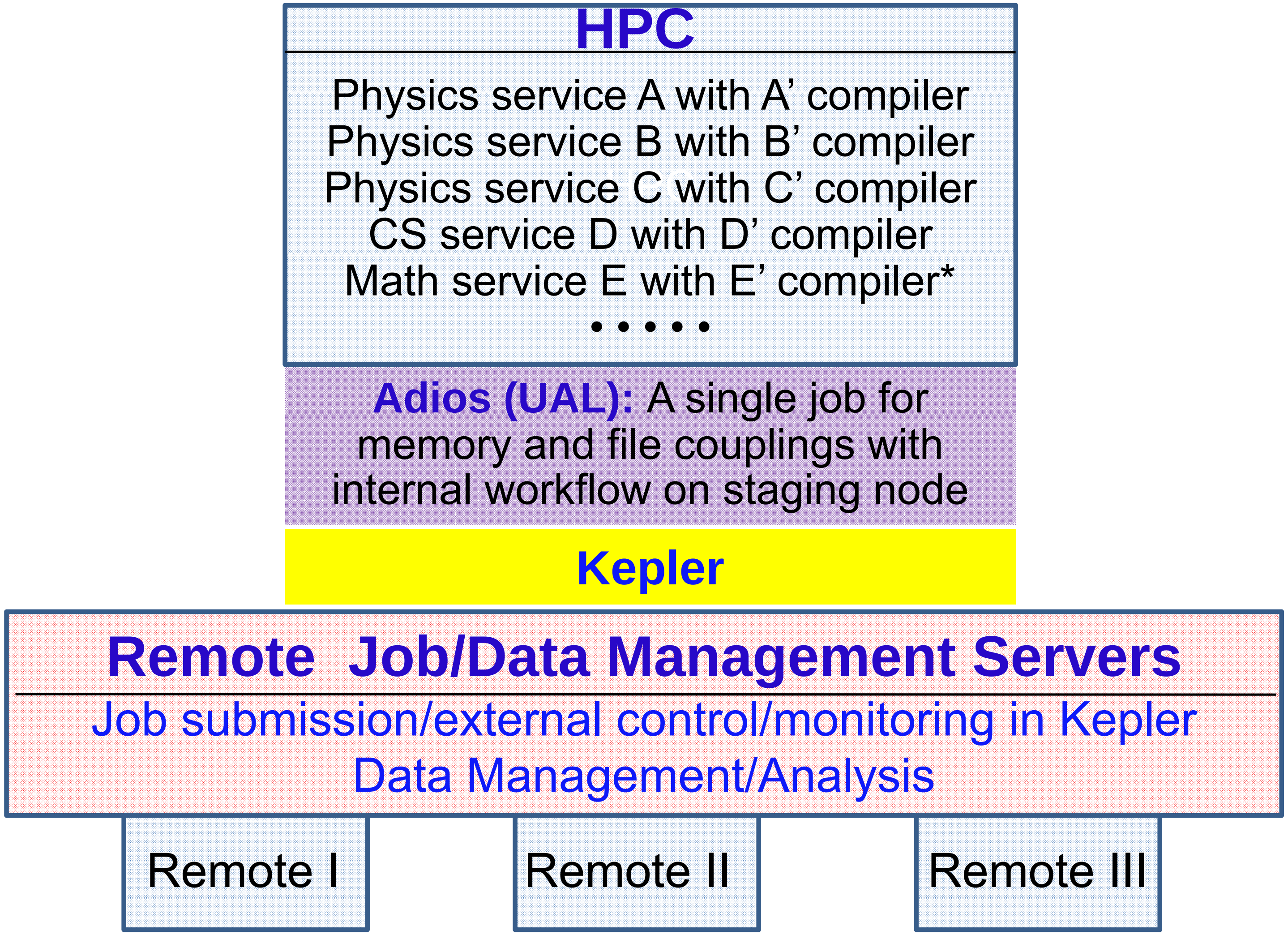
Status of multiscale code Integration in CPES on EFFIS framework (1 day run goal, Nonlinear MHD is bottleneck)



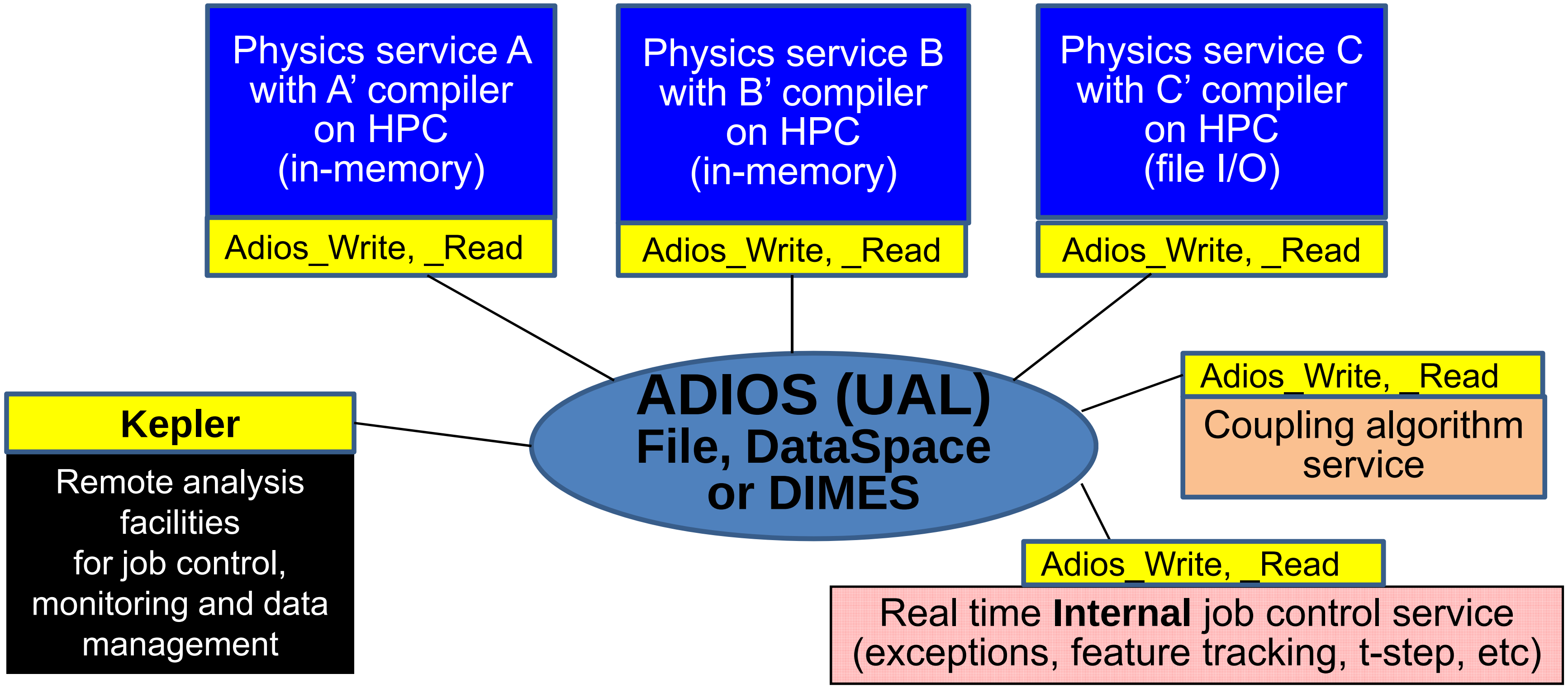
Shift of target hardware system for EFFIS



EFFIS Design in Service Oriented Architecture
(End-to-end Framework for Fusion Integrated Simulation)

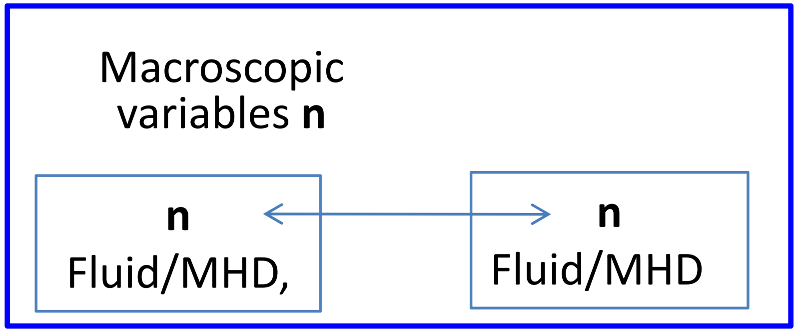


EFFIS framework is a convenient tool-set for SOA code integration (Example)

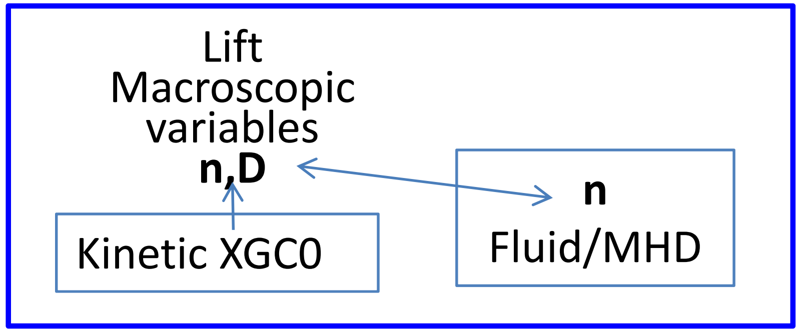


Fast I/O & data movement tools

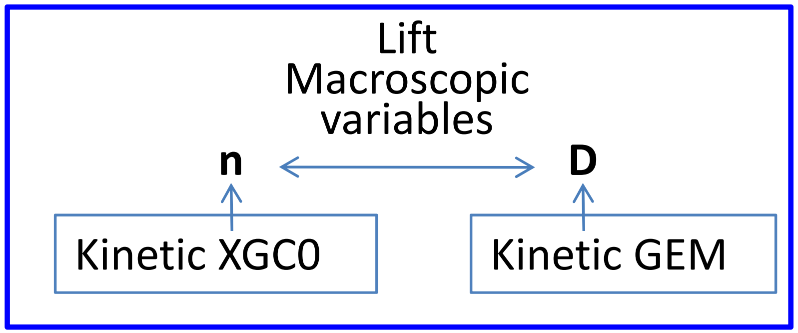
Macroscopic level code couplings in CPES



Type I



Type II



Type III

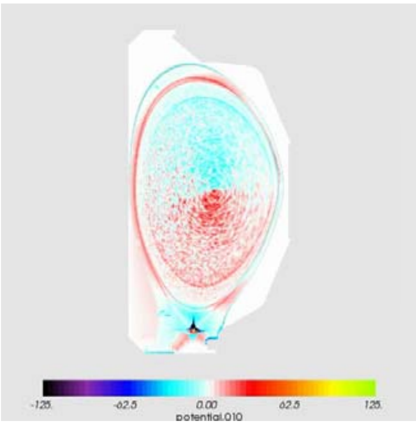
We currently have

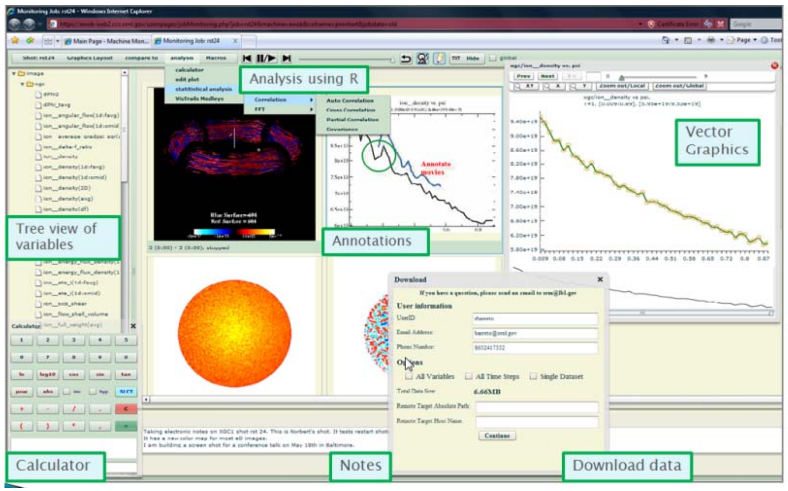
- Weak Type II and III couplings.
- Strong Type II coupling.

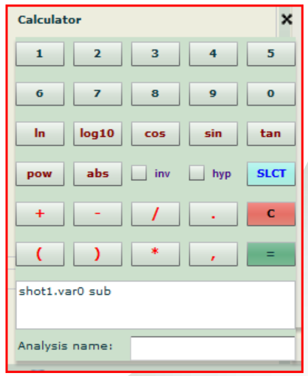
Research Enabled by EFFIS: Example 1

Peta scale simulation of XGC1: Enabled by EFFIS I/O, with real time monitoring of scientific results

- Before Adios, 2Tb restart file was taking > 1 hour for every hour of run on 196,608 process cores (using parallel HDF5).
  - Adios (Adaptive I/O) in EFFIS: ~40GB/s: takes ~ 1minute for 2Tb restart file
- Before EFFIS, the job originator and the collaborators had to wait until the long simulation was finished and/or the large size data is moved before they could monitor/analyze the result.
  - With **Kepler workflow**, **DataMover-lite**, and **eSimMon Dashboard** in **EFFIS**, the job originator and the collaborators can monitor/analyze the data in real time on remote web screen.



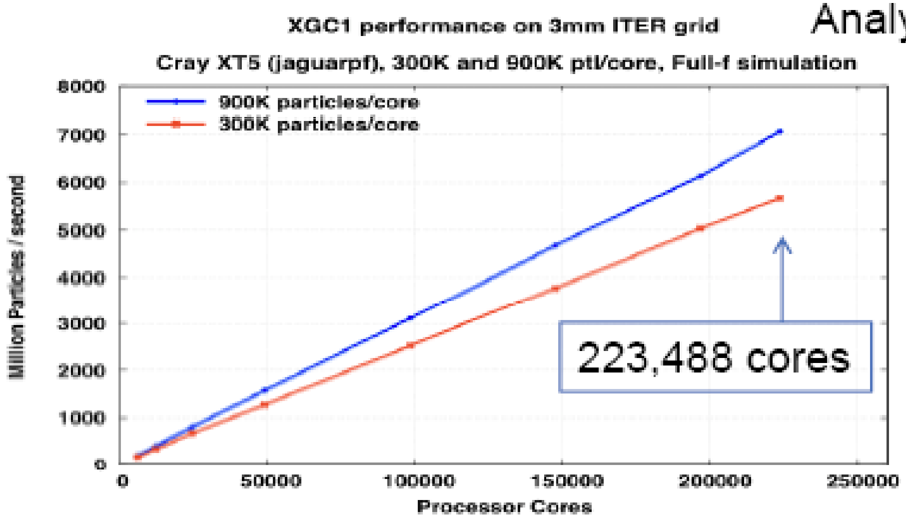


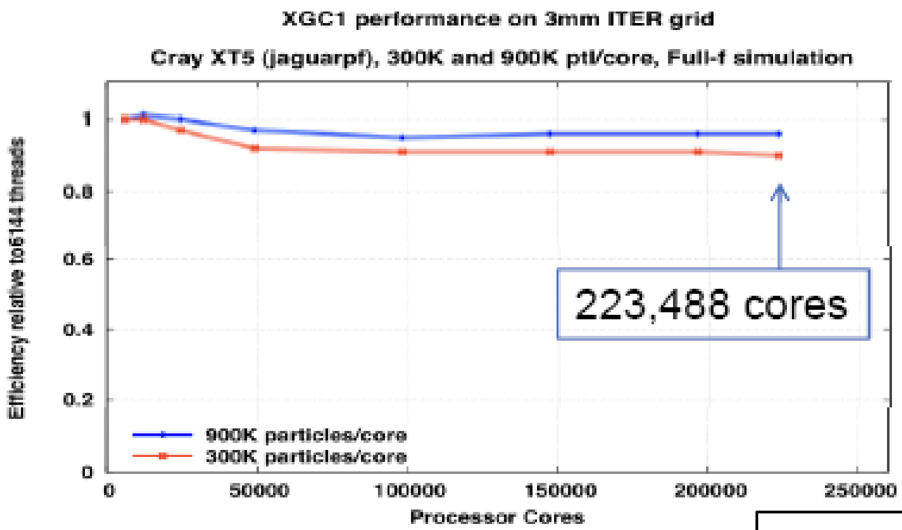


XGC1 scalability and efficiency at two different computational intensity

Best performance achieved with 2 MPI processes per node (12 cores per node)

Analyzed by P. Worley: worleyph@ornl.gov

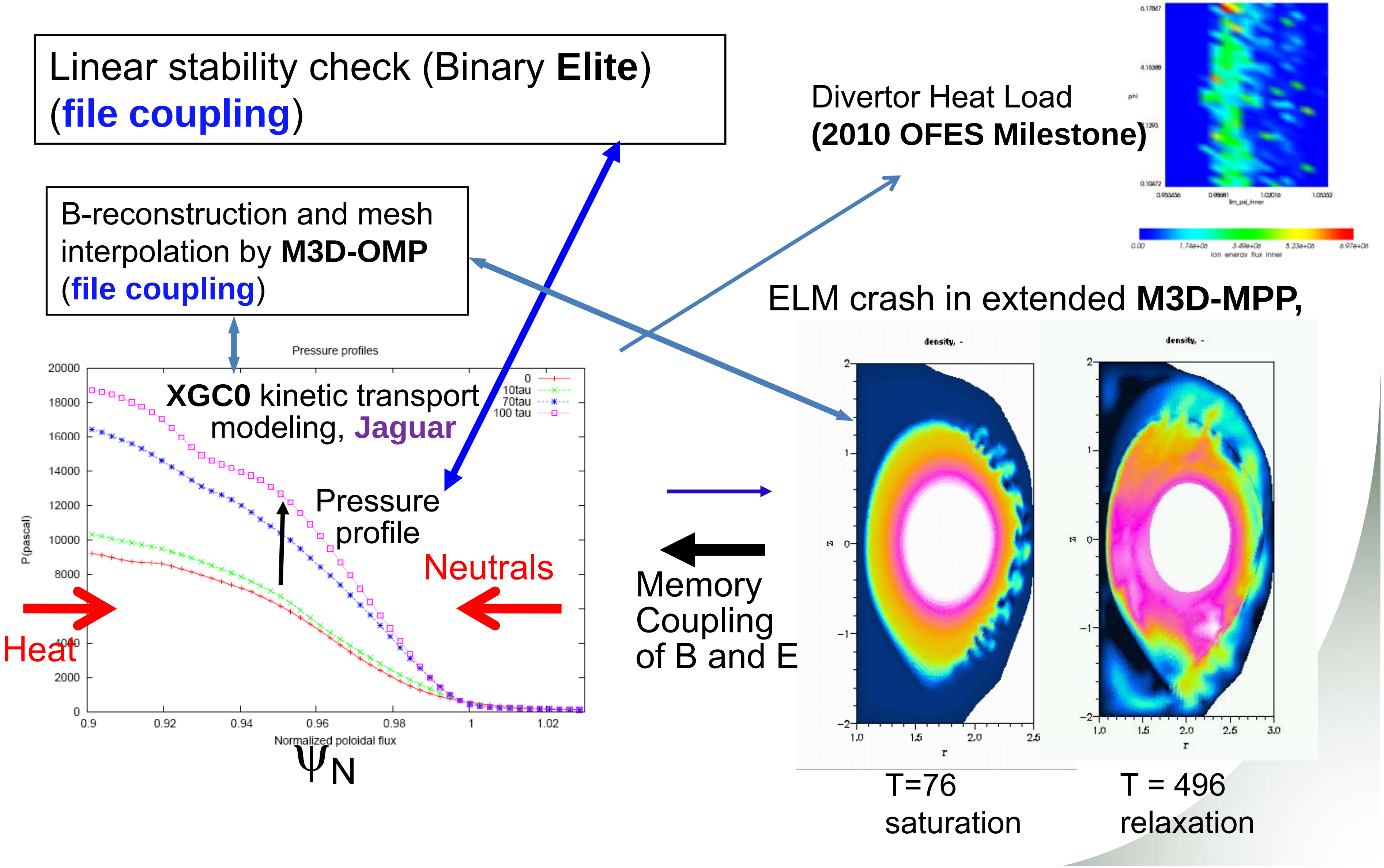




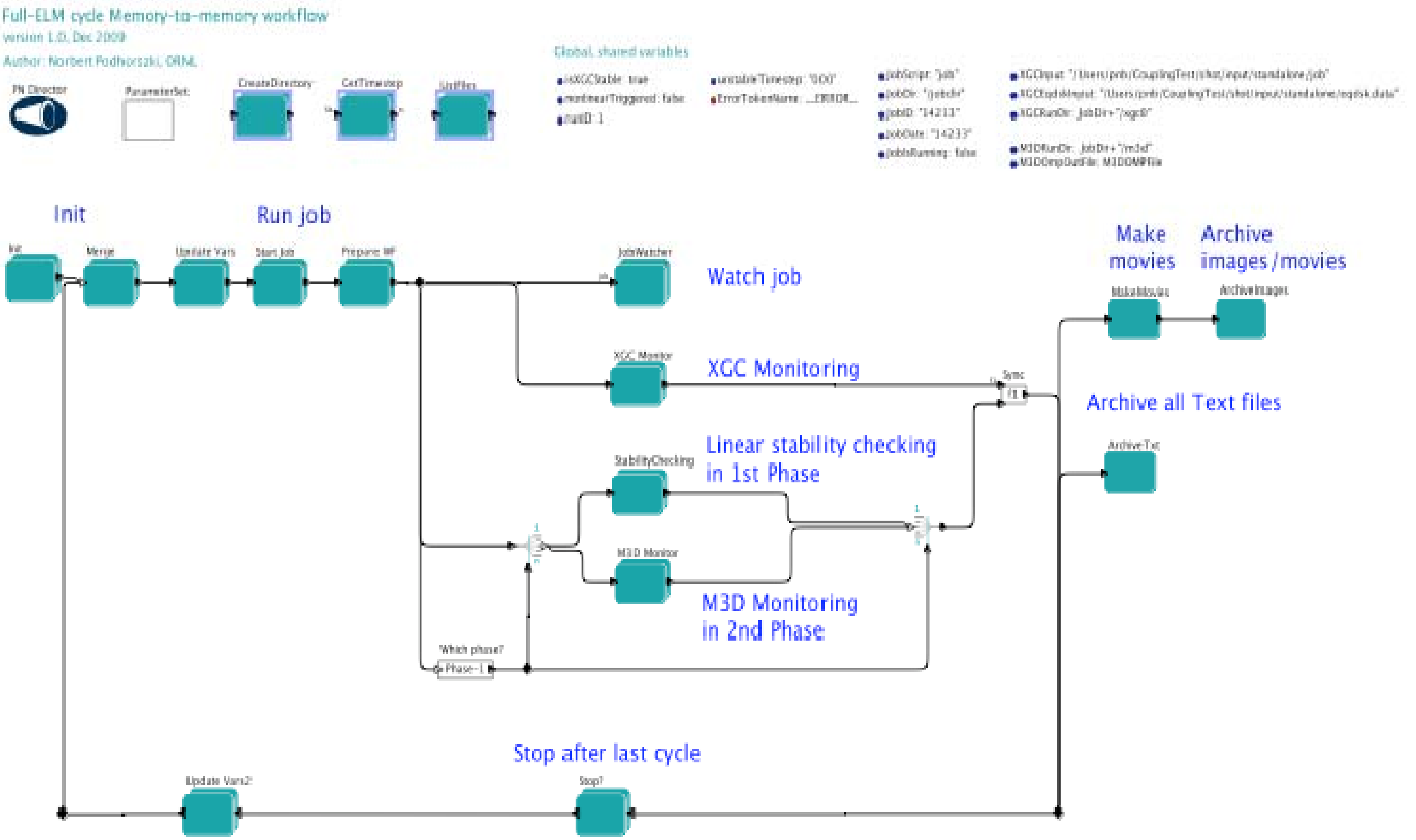
- 900K particles per thread problem is more computationally intensive than 300K problem, which leads to a somewhat higher particle push rate (approx. 20%).
- Particle number per thread will decrease to 300K in the future, as demanded by the memory/thread decrease in the future hardware architecture.
- **Performance scaling is excellent for both problems.**

→ Stronger inhomogeneous computing

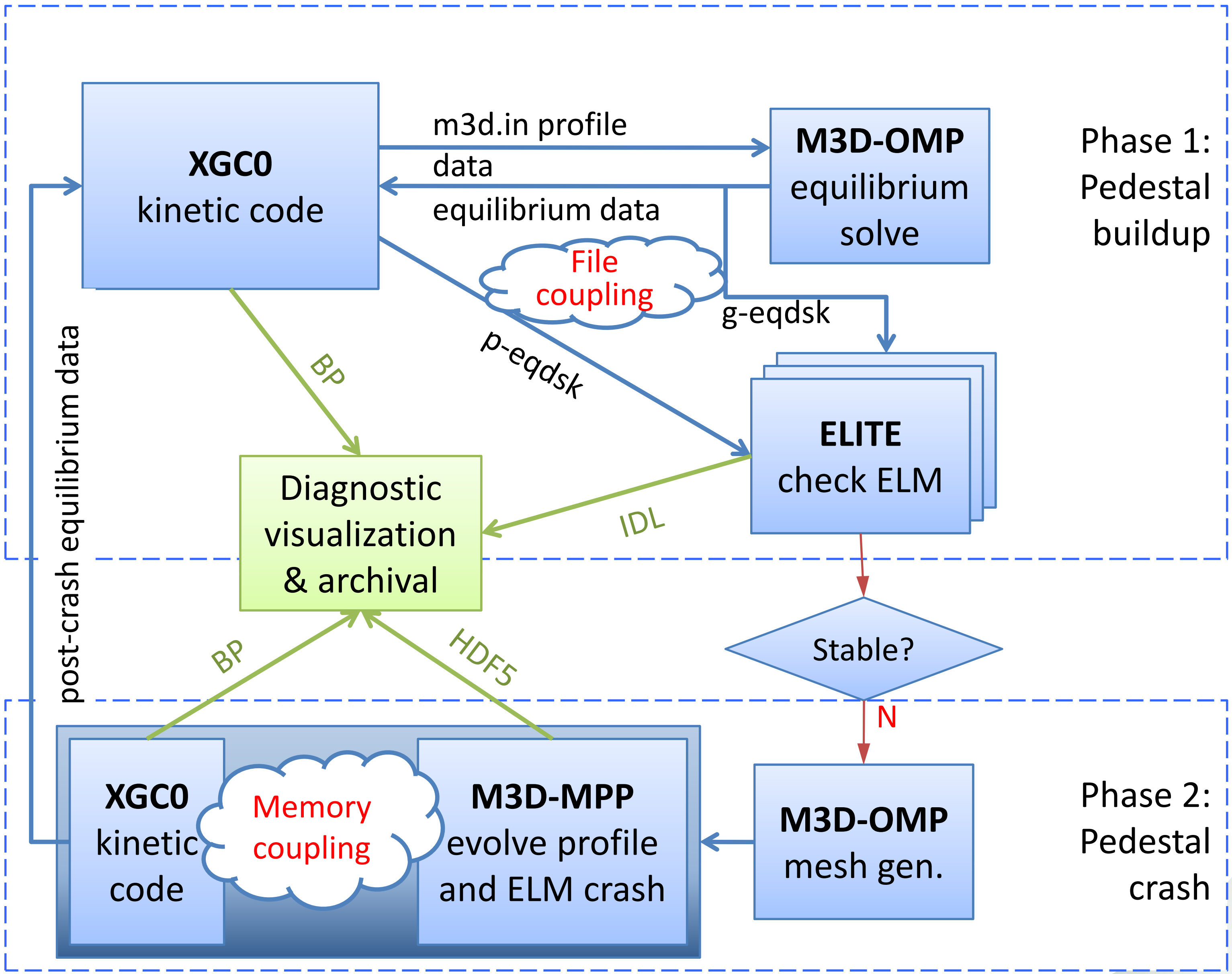
Example 2: Weak coupling between particle and PDE codes: Kinetic-MHD coupled simulation for pedestal-ELM cycle in automated EFFIS framework



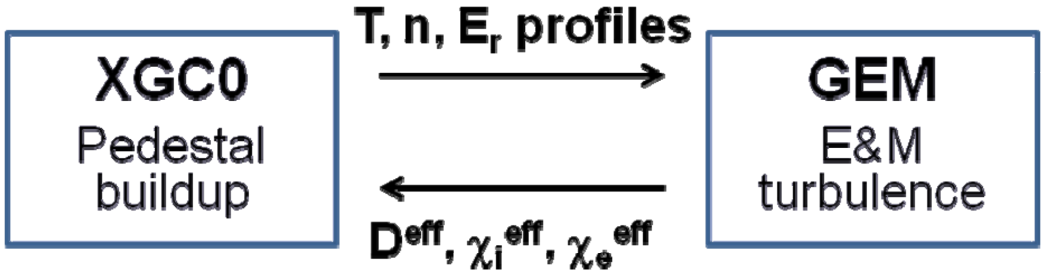
In-memory Coupling workflow for ELM cycle



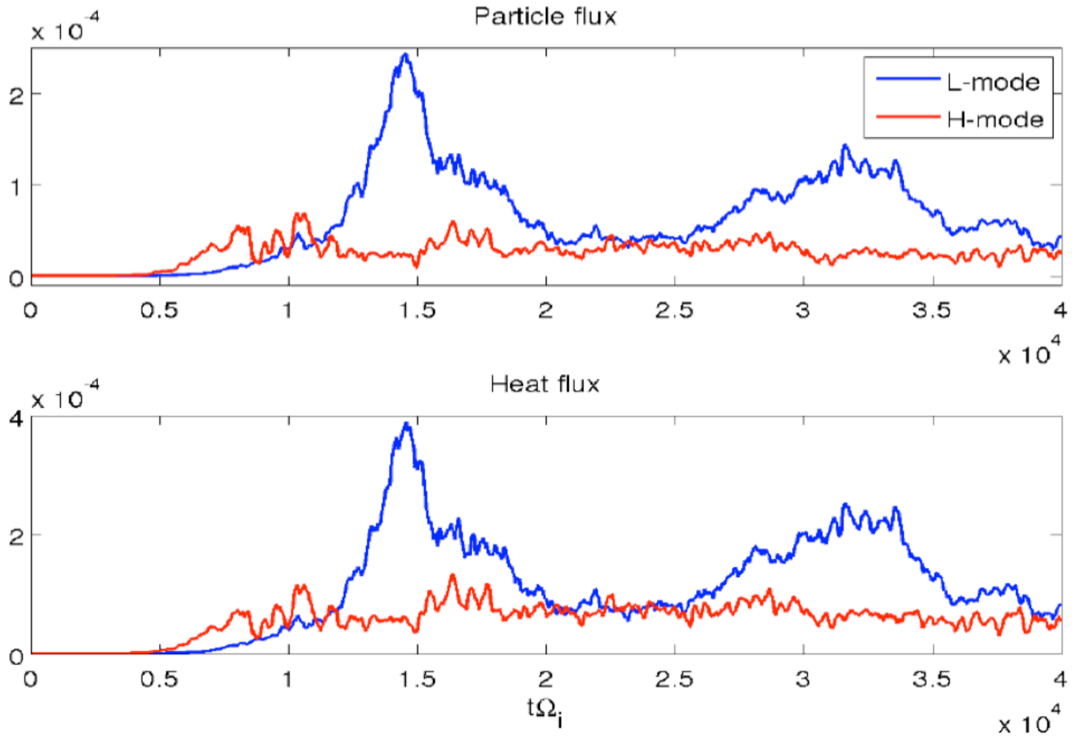
Full-ELM coupling scenario (divertor heat-load study)



Example 3: Weak coupling between particle and particle codes (XGC0 and GEM) for preparatory study of electromagnetic turbulence transport during the edge pedestal evolution (before the XGC1 coupling)



GEM imports a radial section of XGC0 plasma inside the magnetic separatrix surface



Particle and ion heat fluxes in L- and H-mode XGC0 plasmas with a DIII-D Experimental magnetic equilibrium.

Example 4: Strong coupling between particle and PDE codes to study RMP penetration and pedestal evolution

XGC0 evolves plasma profiles under new δB and calculates new perturbed current $\delta J_{||}$.

$\delta J_{||}$ ⇨

⇦ $\delta\vec{B}$

Solver code calculates new 3D δB from perturbed current $\delta J_{||}$ evaluated in XGC0

- Solve two coupled systems

$\delta j_{||}/B = F(\delta\psi)$: Vlasov-Poisson system (XGC0)

$\Delta^{*}\delta\psi = \mu_0 \, I \, \delta j_{||}/B$: Perturbed magnetic field solver.

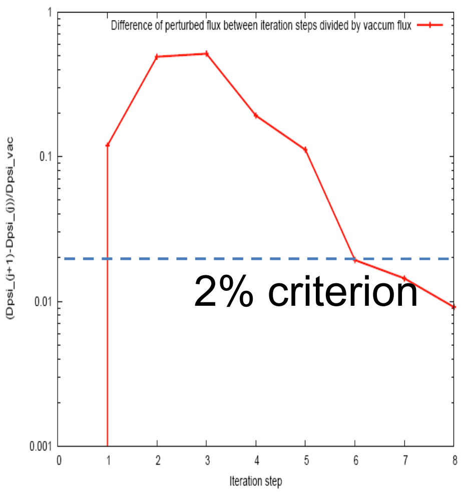
- Use damped iteration scheme

$$\delta\psi_{k+1,(m,n)}(r_i) = \delta\psi_{k,(m,n)}(r_i) + s_{(m,n)} \, \Delta\psi_{k,(m,n)}(r_i)$$

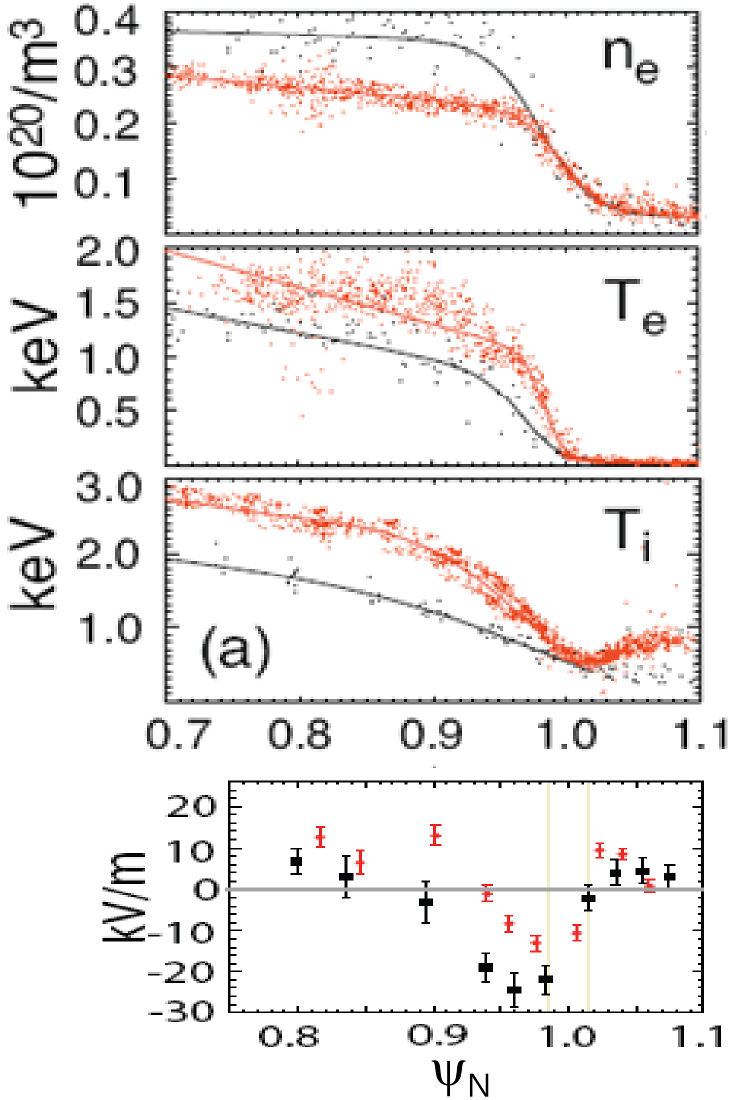
$$s_{(m,n)} = \mathrm{Min}_{r,m} \, [1, \alpha \, \mathrm{Min} \, (|\delta\psi_{k,(m,n)} / \Delta\psi_{k,(m,n)}|)]$$

$\Delta\psi_{k,(m,n)}$ is the correction of $\psi_{k,(m,n)}$ at the k-th iteration step

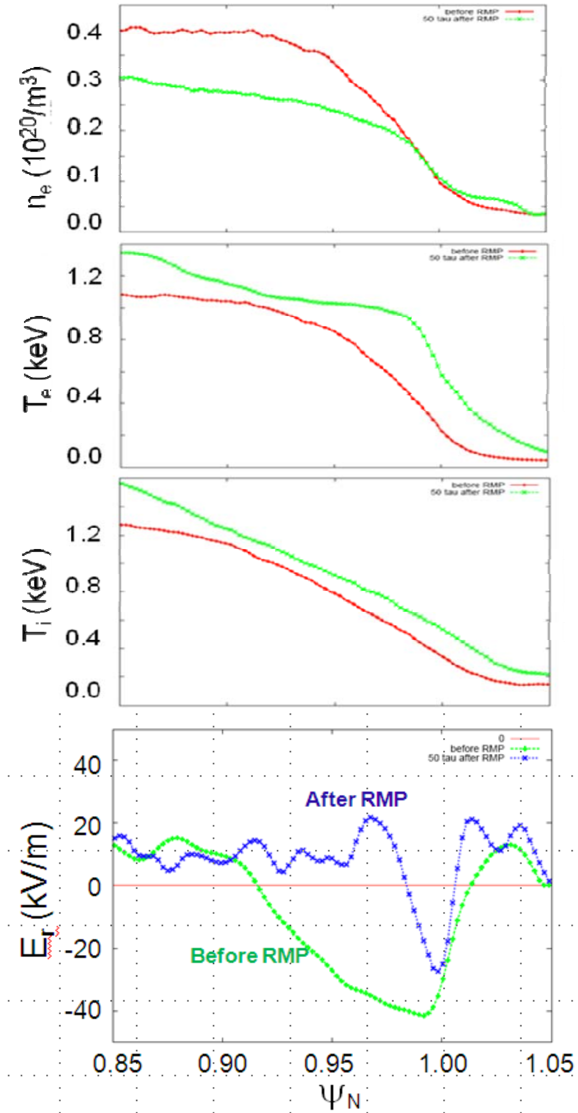
- Converged solution with the criterion $\Delta\psi / \delta\psi_{vacuum} < 2\%$ is obtained in 7 iterations for the case studied here.



Validation with DIII-D experiment

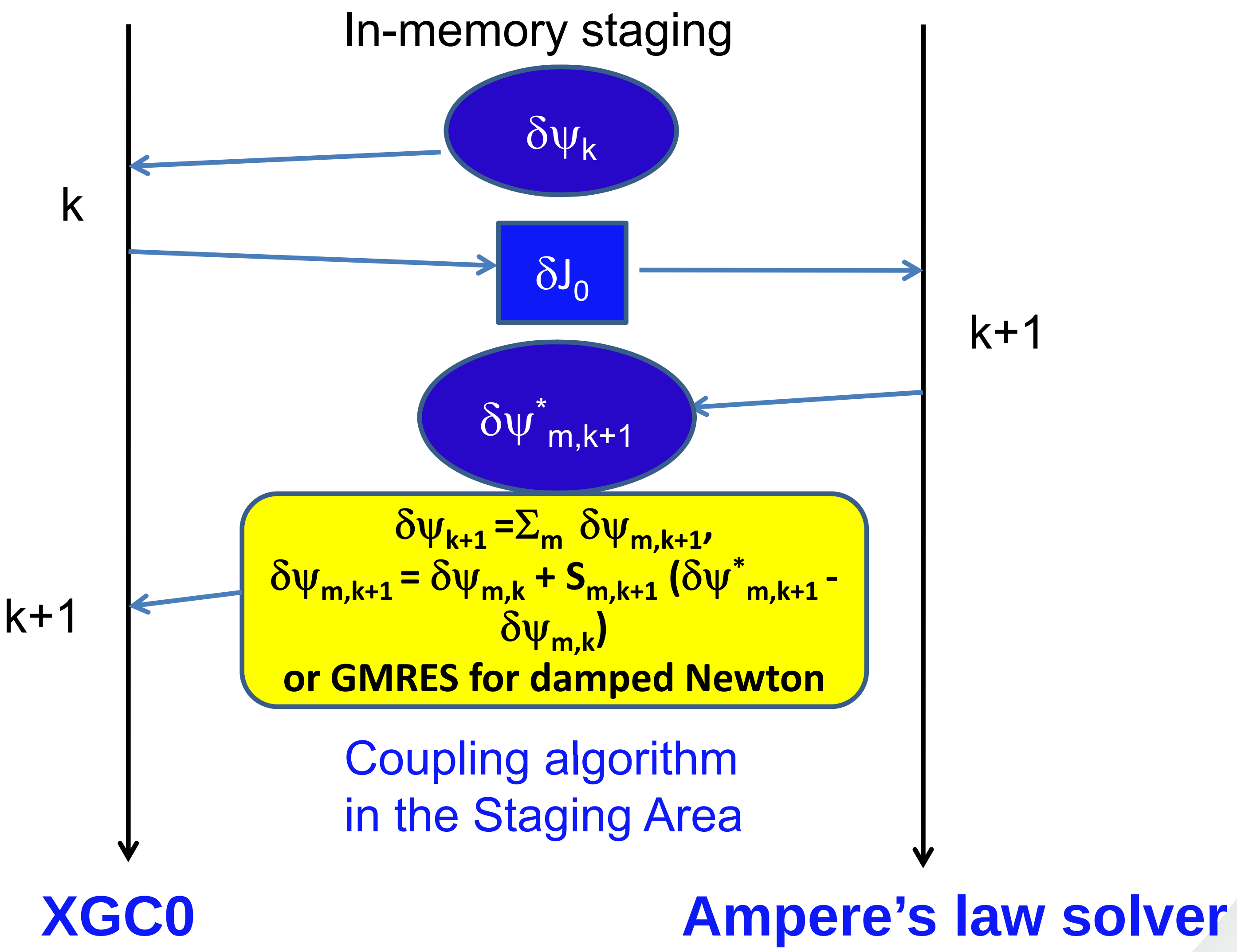


DIII-D Experiment 126006. Black is before and red is after RMP turn-on.



Simulation. Red is before and green is 4ms after the RMP turn-on..

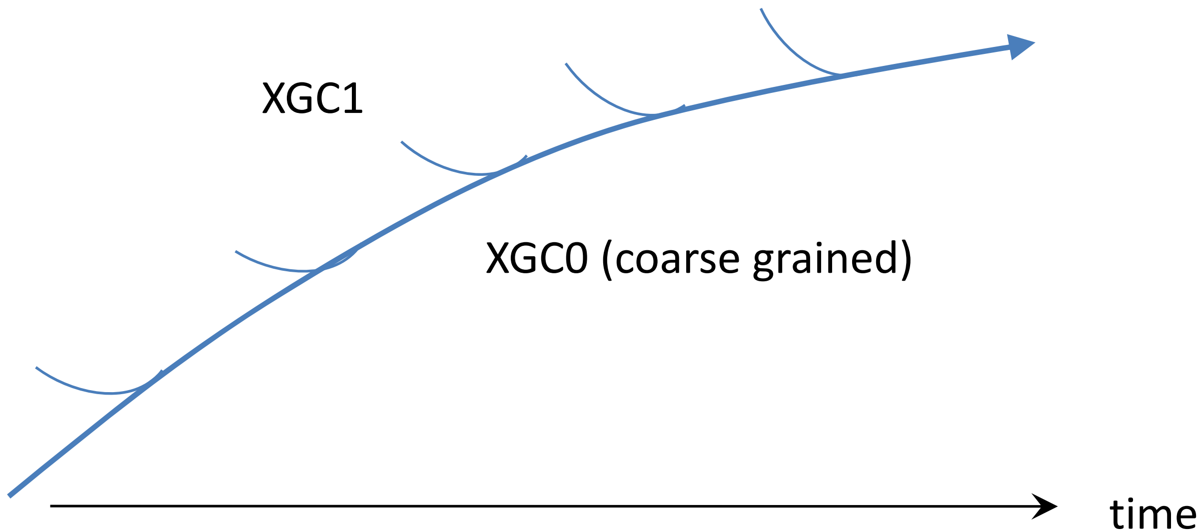
Strong Coupling: Damped Iteration Solution on EFFIS/Adios



Kinetic level code-coupling research in CPES without lifting to the macroscopic variables

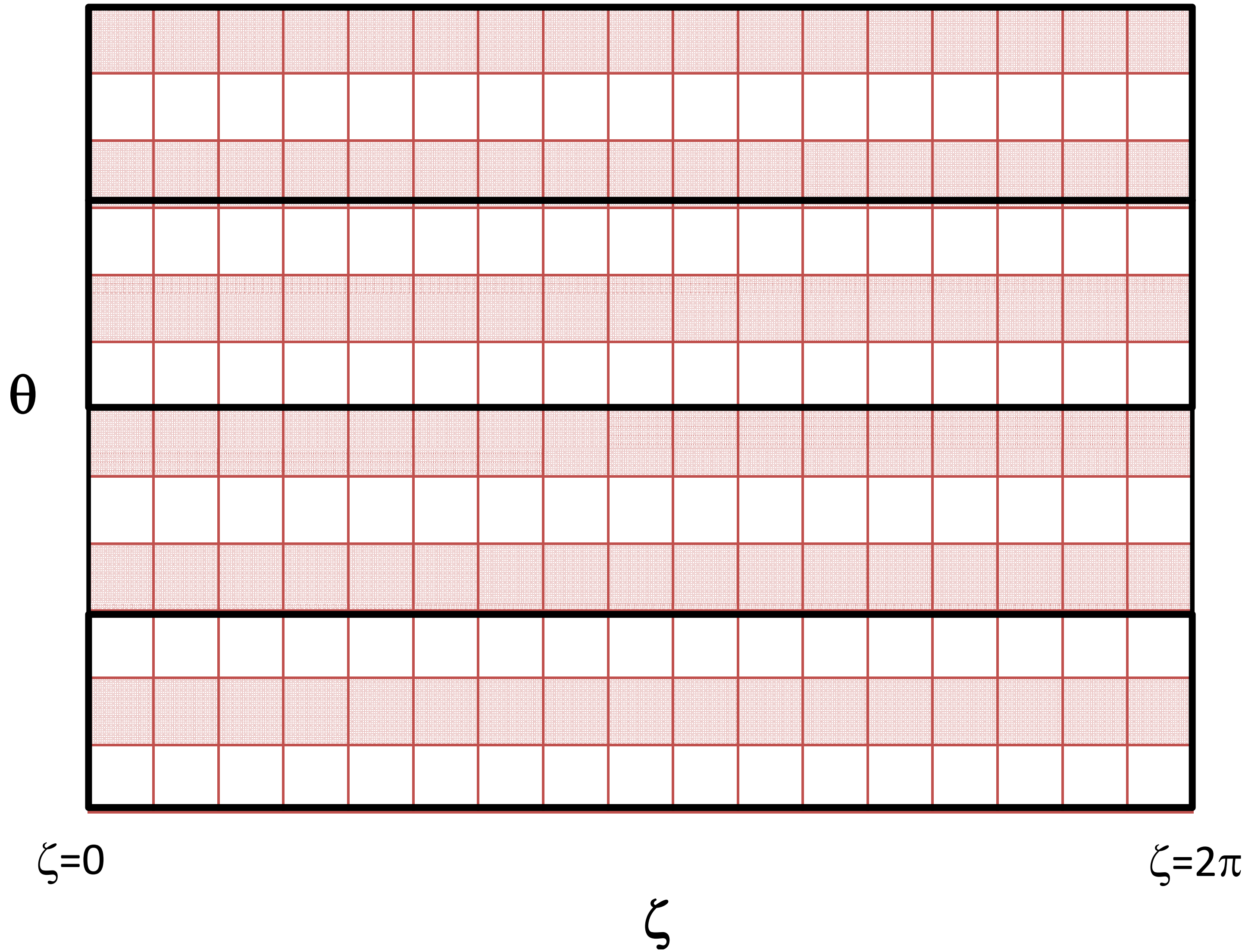
In order to enable experimental time-scale kinetic simulation with XGC1 kinetic turbulence capability and XGC0 kinetic transport model capability, we are conducting pineering research on projective integration scheme on the coarse-fine graining operations (lifting/prolongation-restriction) within the XGC1 code.

Use Adios workflow.



This coupling technique is to be extended to second order.

Grid coarsening and refining for lifting and restriction



Conclusion and discussion

- EFFIS (**End-to-end** Framework for Fusion Integrated Simulation) is a comprehensive **single-framework** approach to code integration for file and in-memory couplings; which can include the run-time functionalities such as job submission, monitoring, job control, data movement and analysis, provenance capturing, etc.
- EFFIS uses the well-established enterprise technology "Service Oriented Architecture," which embraces
  - Diverse code properties
  - Diverse physics, including nonlocal nonlinear physics
  - High scalability, pushing the edge of LCF
  - Independent development of component codes while connected to the framework
  - Choice of different compilers and library versions for each components
  - Straight forward addition of new tools (or replacement)
- EFFIS purposely does **not** rely on "far out" or "costly" technologies
- Applied to weak coupling in PDF-PDF, Particle-PDF, Particle-Particle; and strong coupling in Particle-PDF codes