

Exascale Computing and Whole Device Model for Fusion

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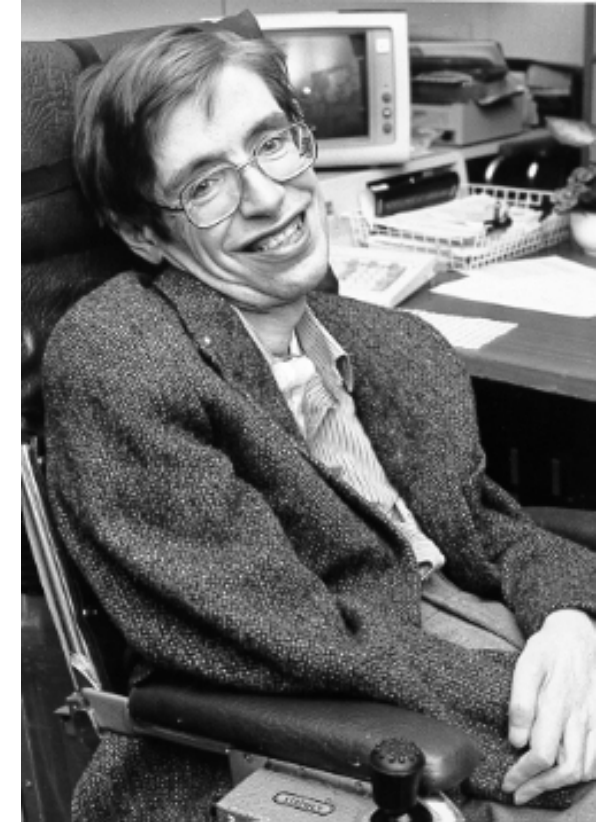
L. Perkins, Project Manager, *PPPL*



EXASCALE COMPUTING PROJECT

Grand Challenge : *Integration* of the knowledge provided by plasma models to understand, predict, and control the performance of fusion experiments

“I think the...21st century will be the century of complexity. We have already discovered the basic laws that govern matter and understand all the normal situations. We don't know how the laws fit together, and what happens under extreme conditions....There is no limit to the complexity we can build using those basic laws.”----Stephen Hawking

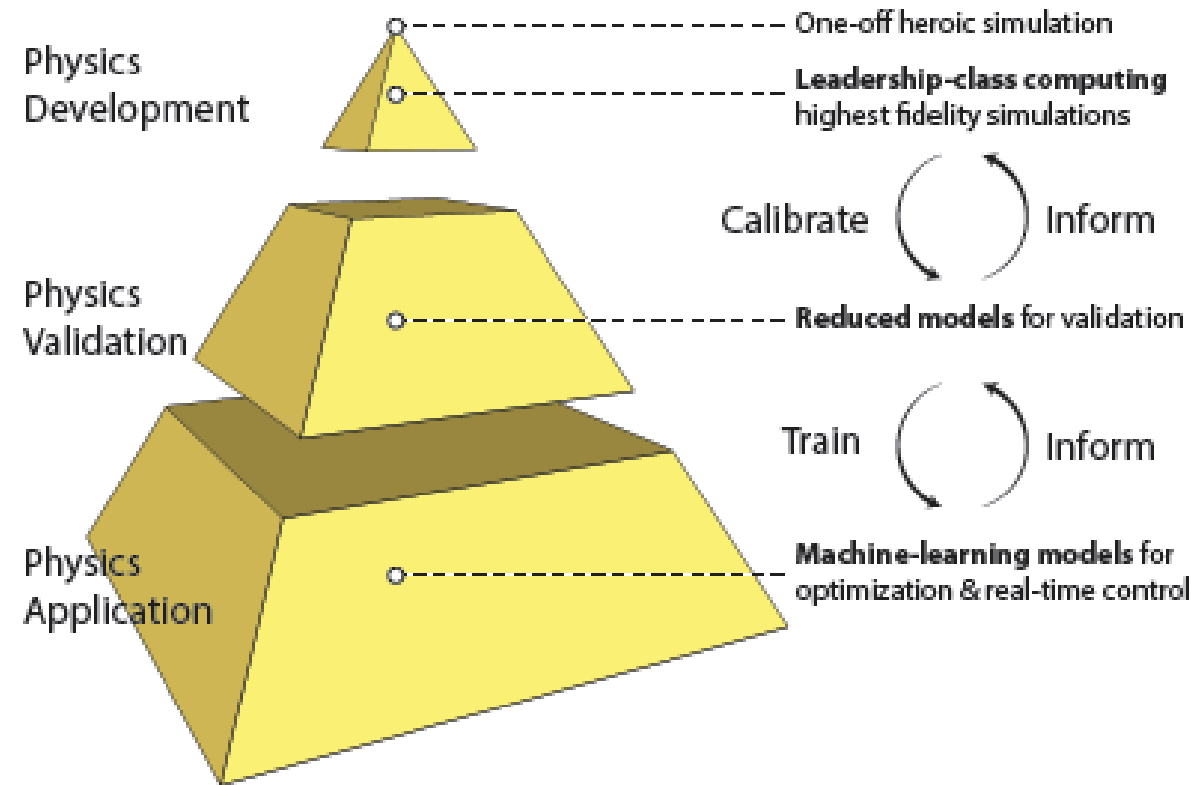


1942-2018

WDM hierarchy: High-fidelity to reduced models

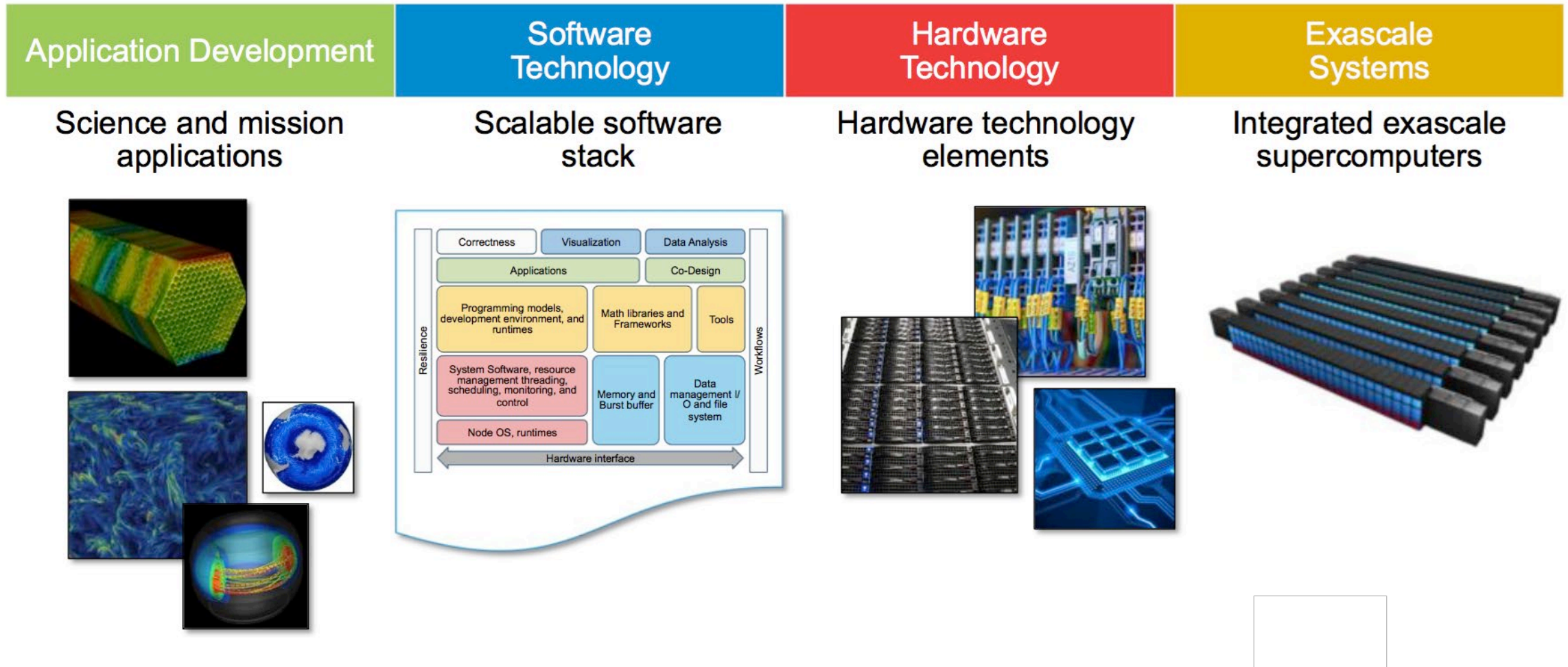
Fidelity Hierarchy is CRITICAL

Range of models from leadership codes to REDUCED MODELS



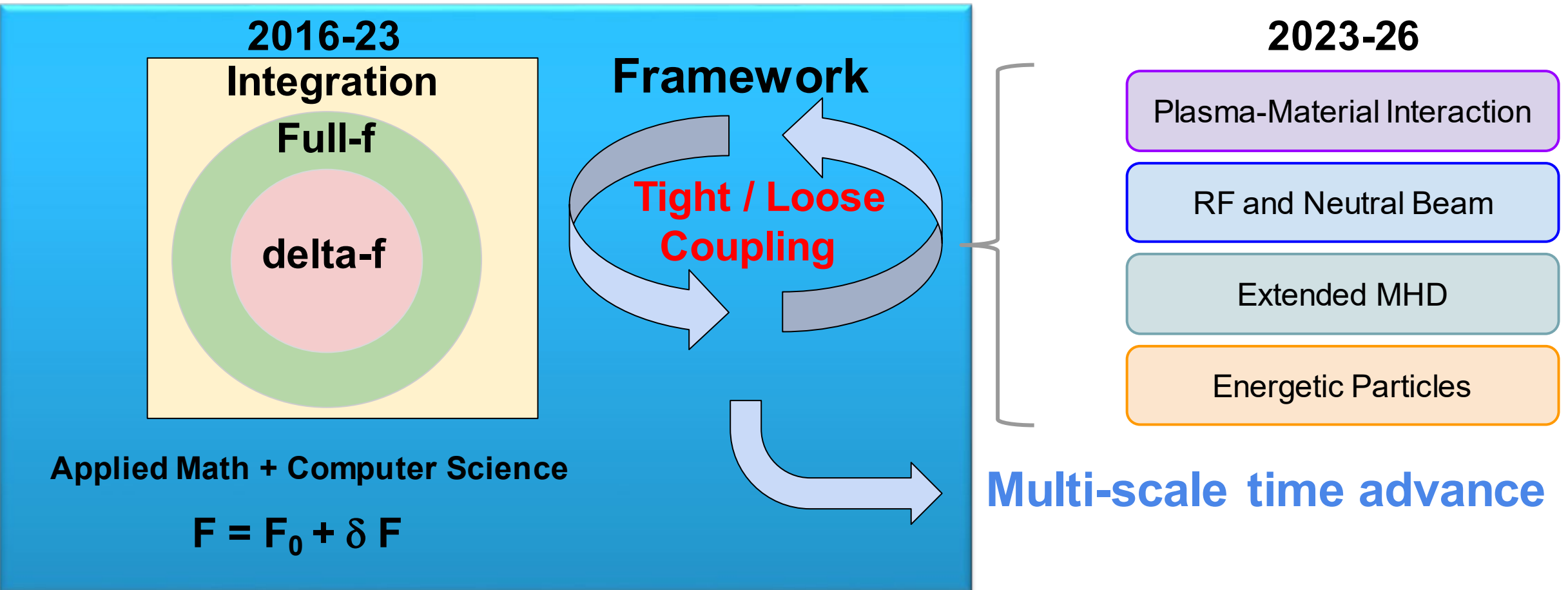
Courtesy: J. Candy

DOE Exascale Computing Program: Holistic Approach (2016-23)



Exascale computers: 10^{18} floating-point operations per second (64-bit floating point precision)

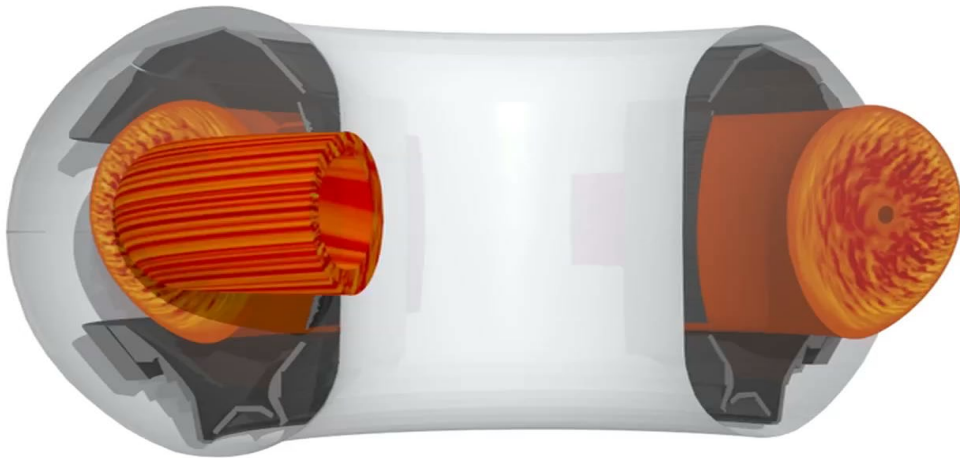
Vision: A High-Performant, First-Principles-Based Whole Device Model



Coupling the core and edge: first in fusion history

The core evolves more slowly than the edge

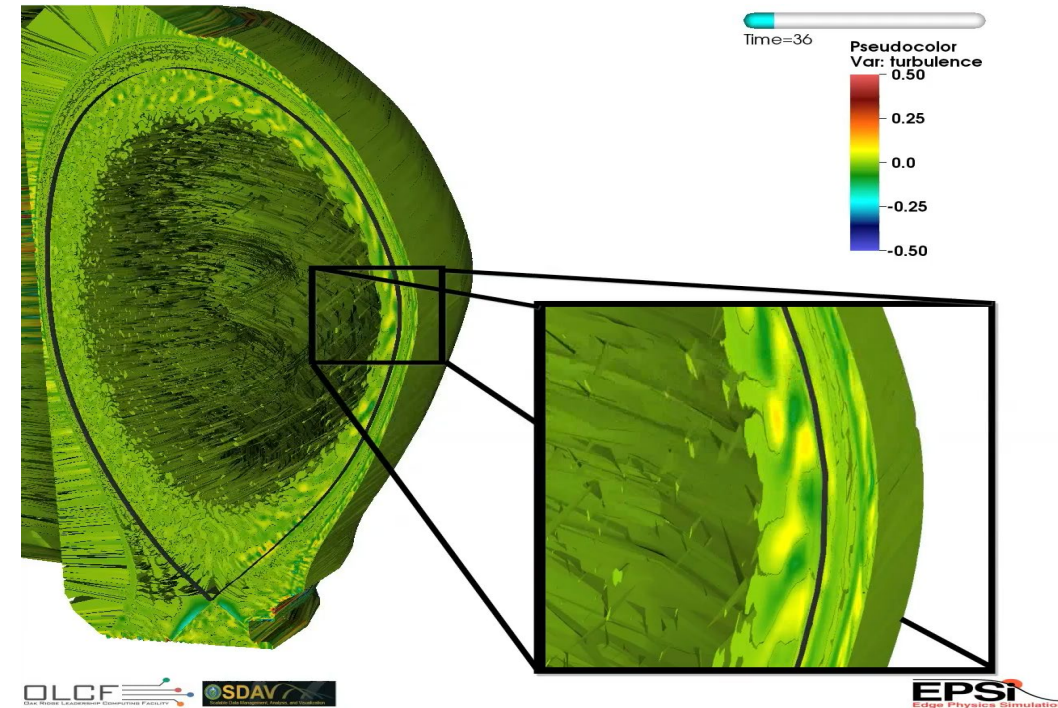
Core Turbulence from GENE



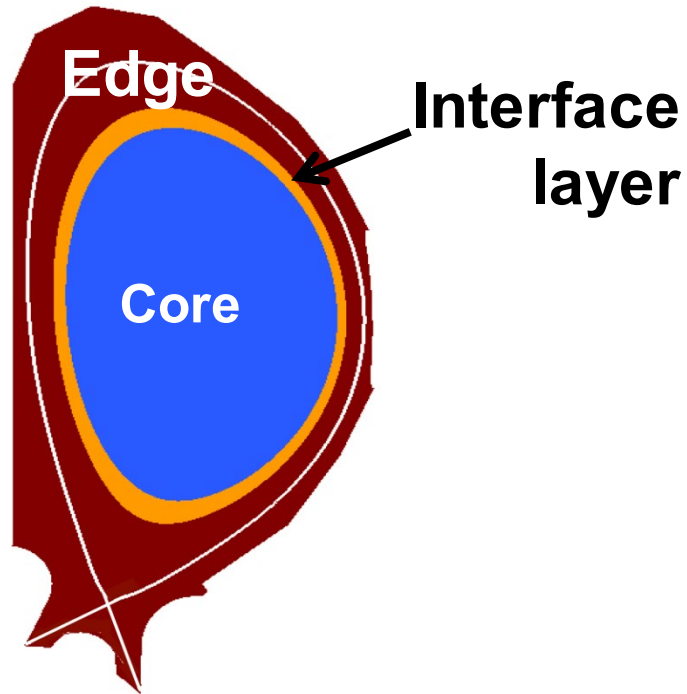
gene.rzg.mpg.de

GENE

Edge Turbulence from XGC



Principal WDMApp Goals

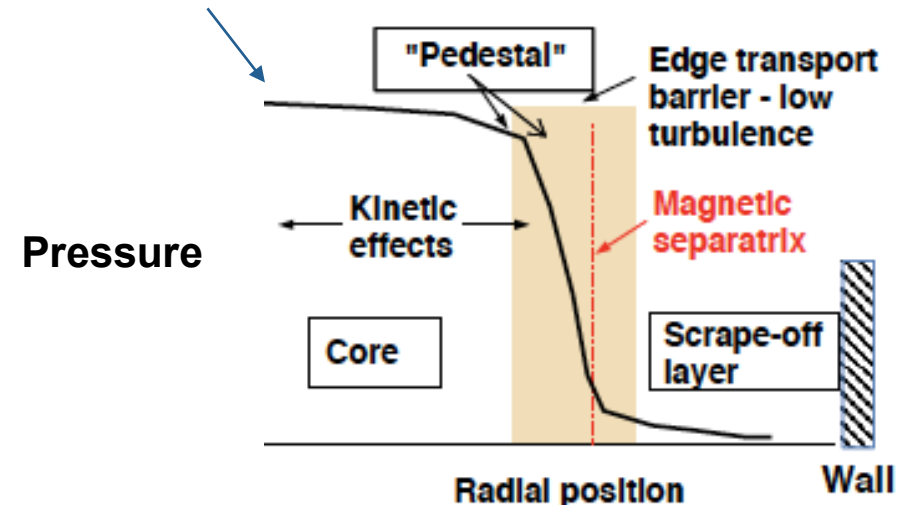
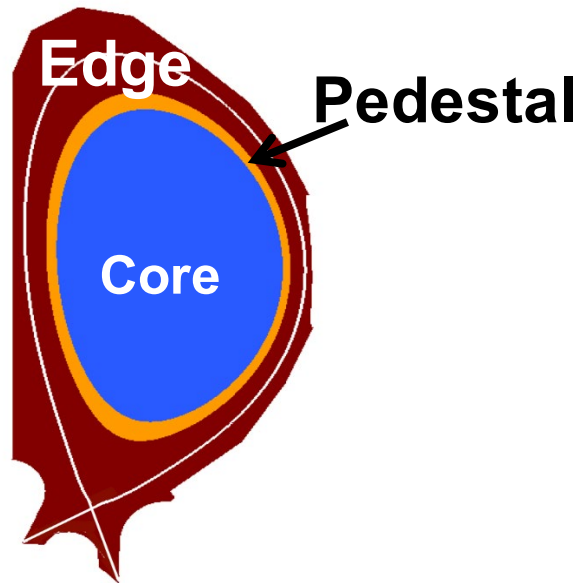


- Demonstration and assessment of WDM **gyrokinetic physics** on experimental transport time-scale in a challenge problem for pedestal formation
- **Figure of Merit (FOM) of >50** for coupled code on exascale platforms, accomplished through algorithmic advancement, performance engineering and hardware improvement
- Completion of **extensible integration framework** EFFIS 2.0 (End-to-End Framework for Fusion Integrated Simulations 2.0) and demonstration on exascale platform

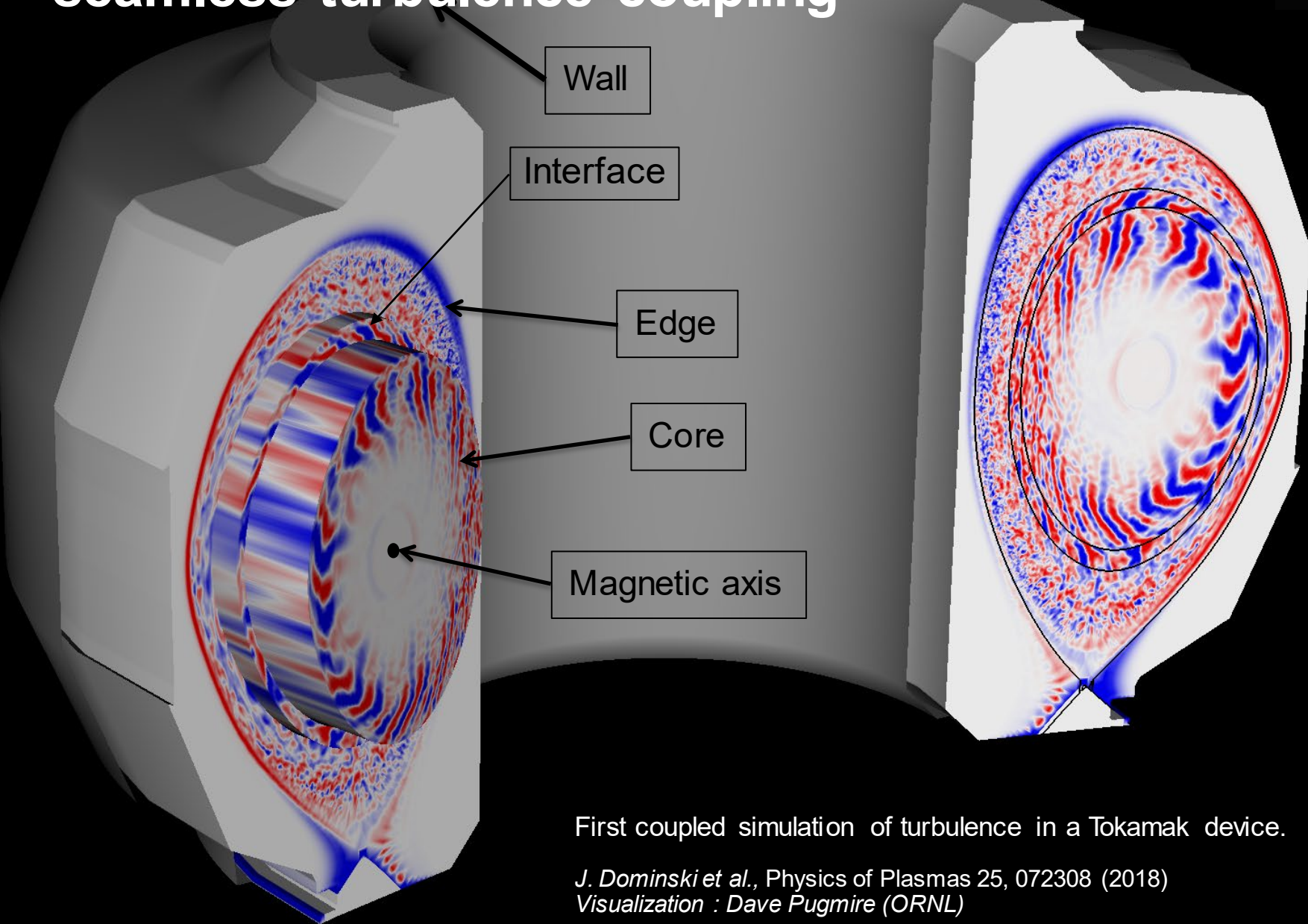
WDMApp Challenge Problem

High-fidelity simulation of a whole-device burning plasma (specifically, ITER with full plasma current) operating in “high-mode” (H-mode), and prediction of the plasma pressure “pedestal” shape (height and width)

Pedestal determines the plasma pressure, hence fusion yield, in the burning core



WDMApp Core-Edge Coupled Simulation shows seamless turbulence coupling



Developing core-edge coupling of technology

1. We first use XGC-XGC coupling to develop the technology
2. Apply the technology to GENE/GEM and XGC coupling

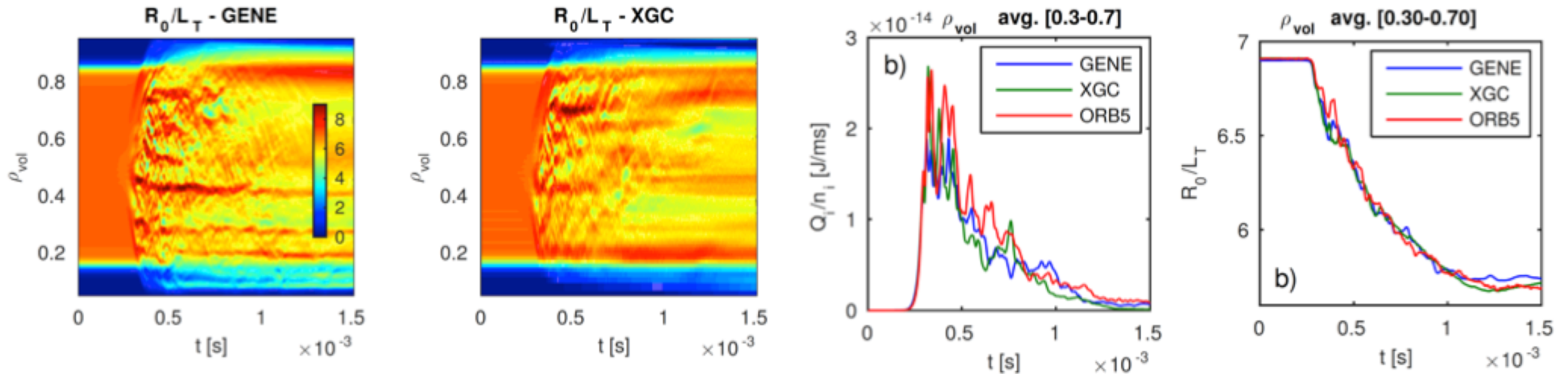
XGC is the leading gyrokinetic code for simulating edge region, including a separatrix.

GENE and GEM are leading gyrokinetic codes for simulating core region.

First coupled simulation of turbulence in a Tokamak device.

*J. Dominski et al., Physics of Plasmas 25, 072308 (2018)
Visualization : Dave Pugmire (ORNL)*

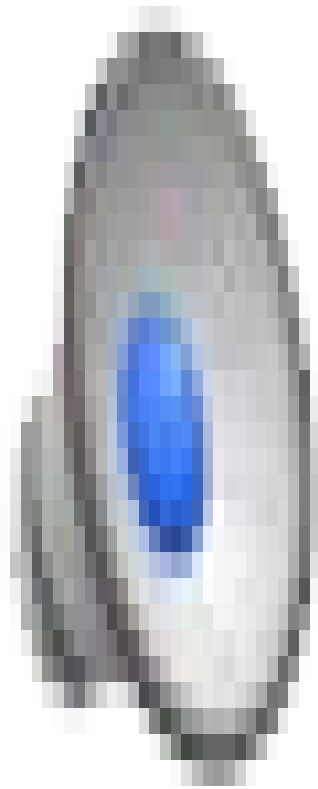
Cross-verification between GENE and XGC: Non-linear ITG instability (J. Dominski, S. Ku, G. Merlo, C.S. Chang, F. Jenko, S. Parker)



Time-radius dynamics of the logarithmic gradient R_0/L_T

Excellent agreement in the time-evolution of the global ion heat flux and temperature gradient. Radial average is taken over the widest region (0.3-0.7) after removing the simulation-boundary area.

Core-edge coupling

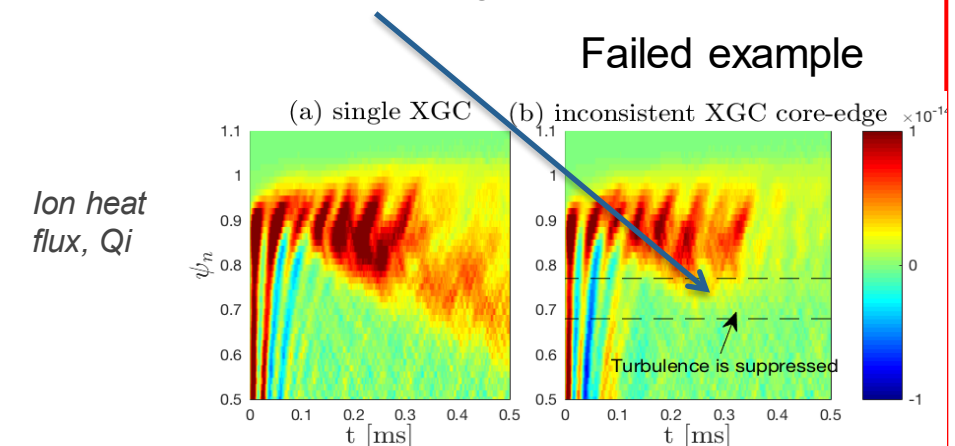


Coupling of XGC-core and XGC-edge

Implemented by J. Dominski, S.H. Ku, and C.S. Chang.

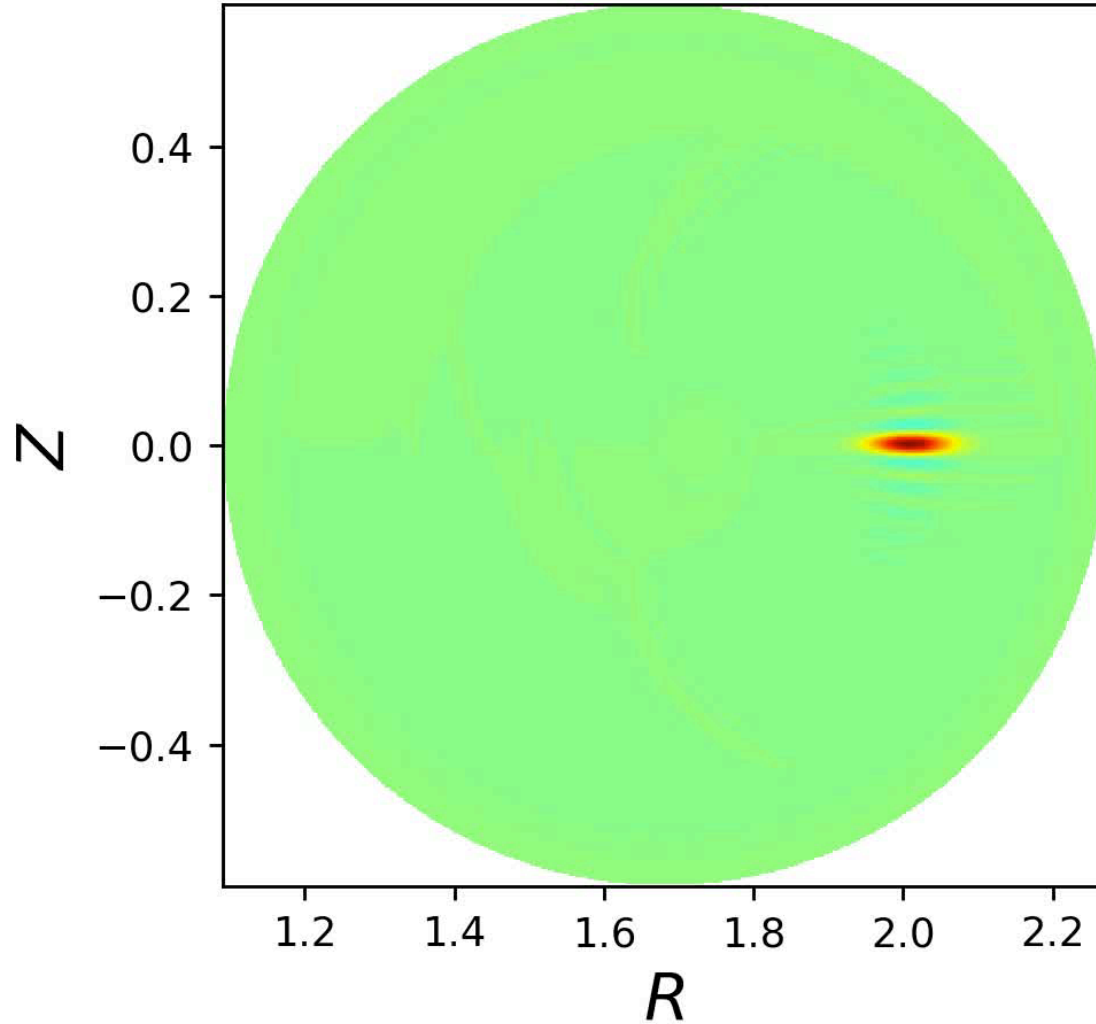
- True kinetic coupling between executables
- The coupled simulation is statistically equivalent to the reference simulation
- Study how to replace the XGC core simulation with a GENE simulation

Difficulty was in avoiding turbulence suppression from nonlinear de-phasing between two codes.

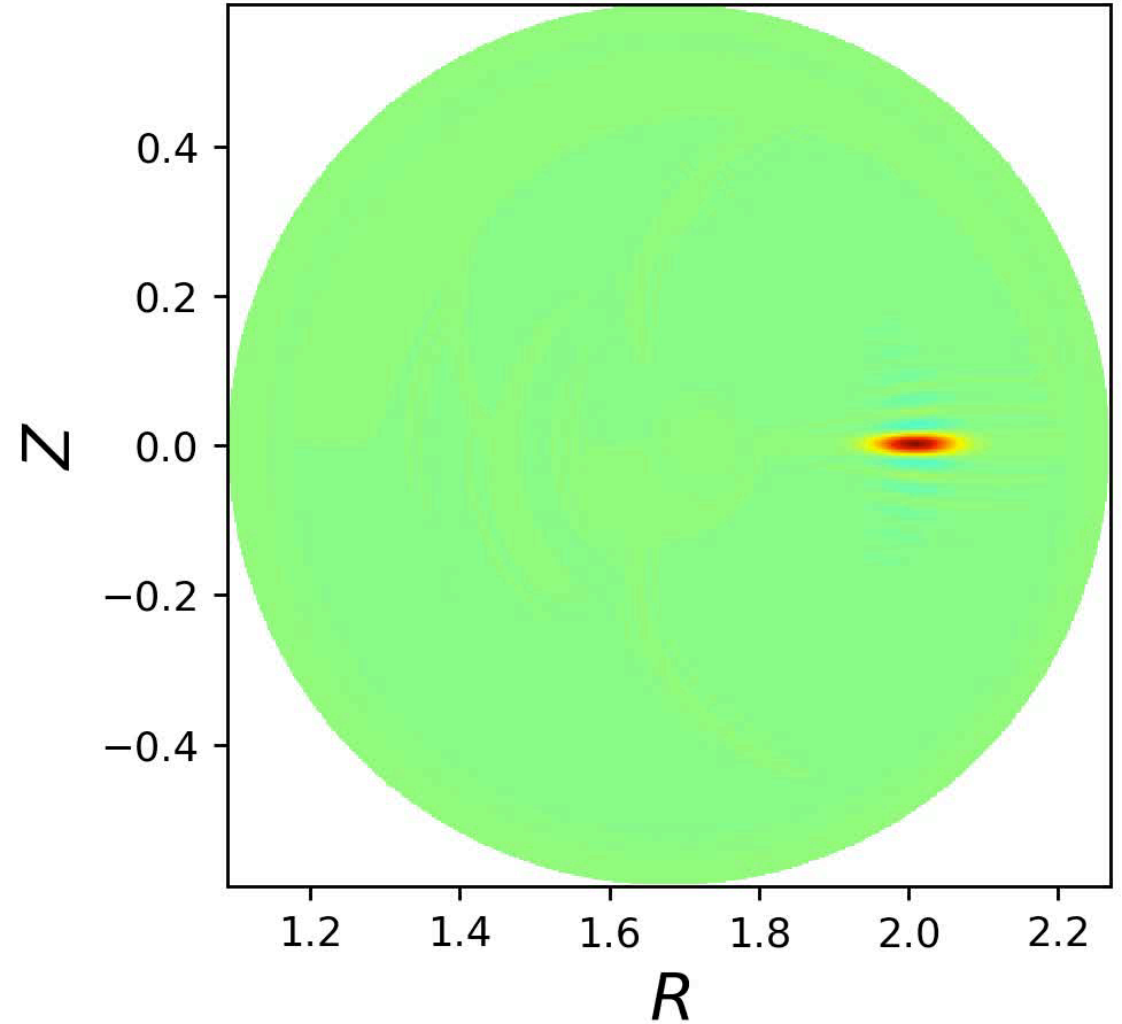


XGC – GEM coupling

ϕ , XGC

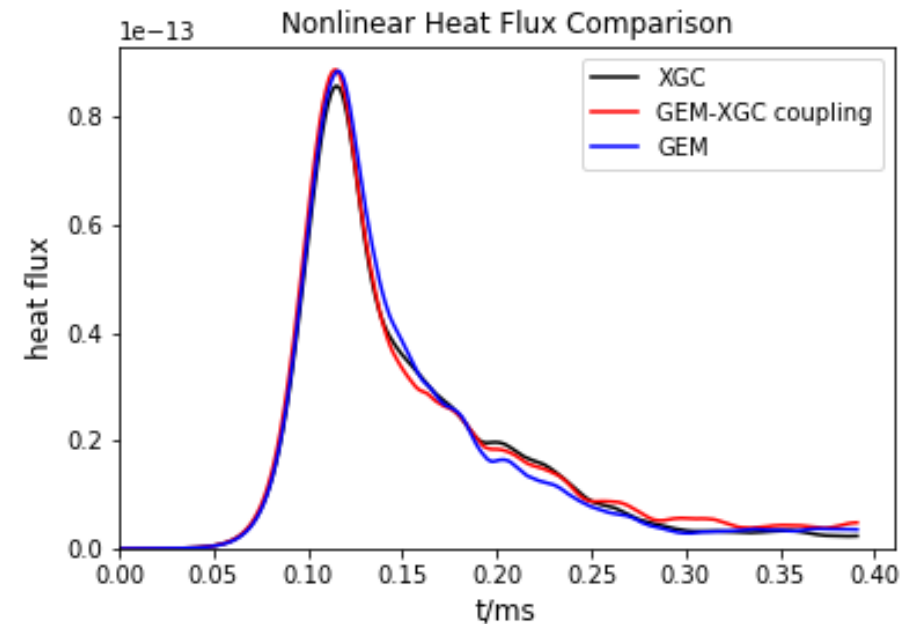
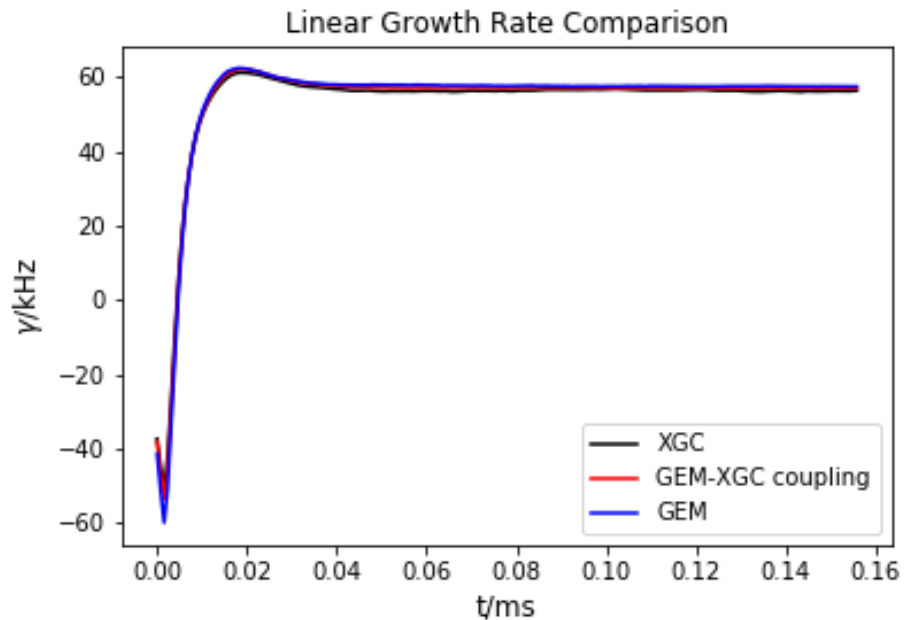


ϕ , GEM-XGC coupling



WDMApp coupling results

- Linear results (n=24): frequency almost the same, growth rate differs ~1%, between coupled code and XGC reference
- Nonlinear results (n=3,6,9,12...) show ~4% difference for the saturation level of heat flux, between coupled code and XGC reference
- Coupled code adds little cost when using parallelized grid-quantity mapping (algorithm and performance enhancement). For example, 24.62s for XGC only, 25.23s for coupling with parallelized mapping.



GENE-XGC Coupling



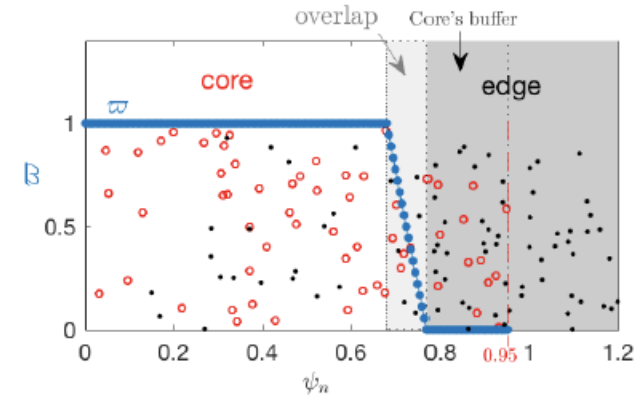
Spatial Core-Edge Coupling

Spatial coupling of gyrokinetic simulations, sharing minimal information

1. In the system of coupled codes, a composite distribution function is used: $f = \varpi f^{Core} + (1-\varpi) f^{Edge}$.

The source term of Poisson Eq. is then computed with

$$\begin{aligned} \bar{n}[\delta\check{f}] &= \int d\mathbf{X} dv_{\parallel} d\mu d\alpha \delta g_c \left[\underbrace{\varpi(\mathbf{X})\delta f^C}_{\text{local in core}} + \underbrace{(1-\varpi(\mathbf{X}))\delta f^E}_{\text{local in edge}} \right] \\ &= \bar{n}[\varpi\delta f^C] + \bar{n}[(1-\varpi)\delta f^E]. \end{aligned}$$



2. Poisson solver needs the exchange of the 3D fields ϕ and \bar{n} between two codes, not the 5D f .

3. The same ϕ will be used in gyrokinetic Eq. (1) for advancing f independently.

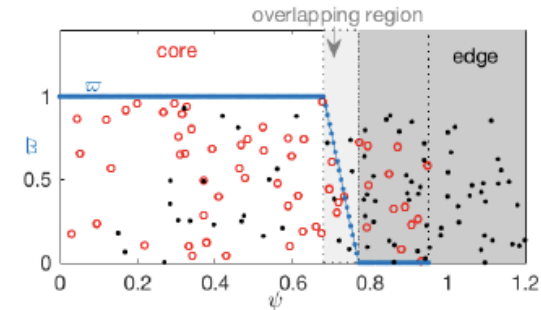
[J. Dominski, et al., Phys. Plasmas **25** (2018)]



Question: Hallatschek

Using a single field solver ensures consistency of the field

Counter example: we tried a simulation using two field solvers and two different boundary conditions.

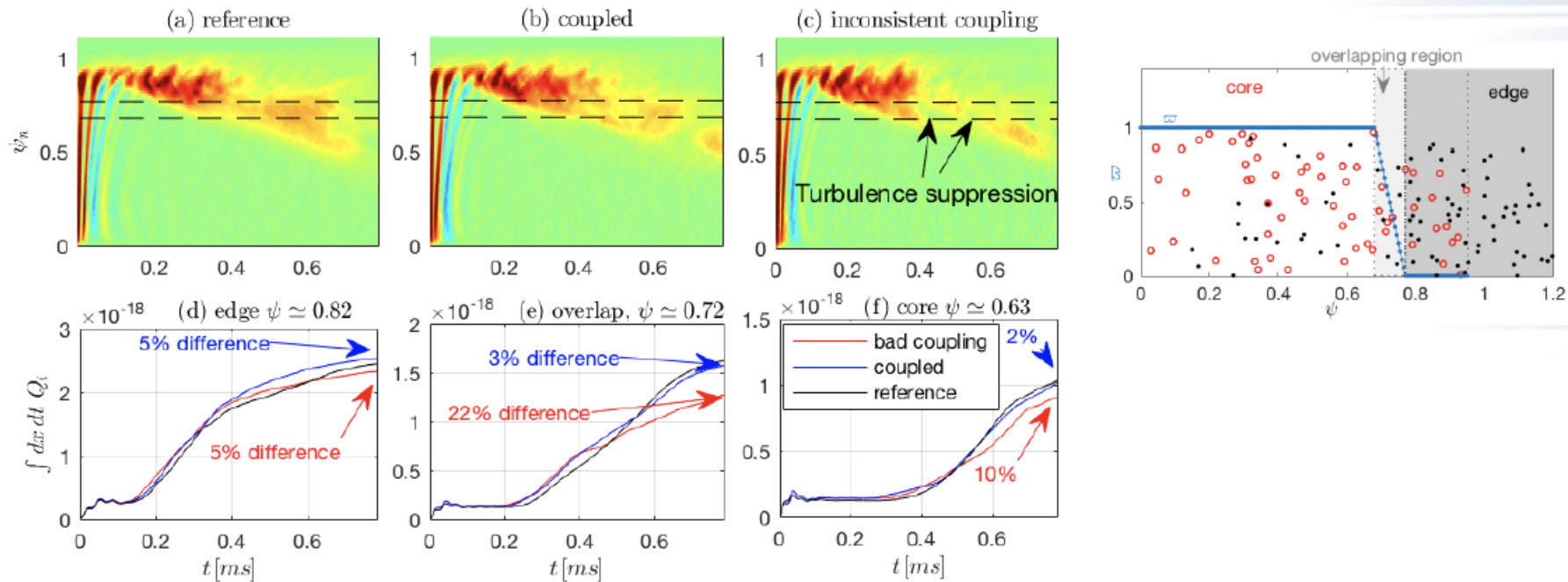


$$\mathcal{L}^C \phi^C = \bar{n}[\varpi f^C + (1 - \varpi)f^E], \quad \psi_n \in [0, 0.95] \quad \text{and} \quad \phi^C|_{\psi_n=0.95} = 0,$$

$$\mathcal{L}^E \phi^E = \bar{n}[\varpi f^C + (1 - \varpi)f^E], \quad \psi_n \in [0, wall] \quad \text{and} \quad \phi^E|_{wall} = 0.$$

\mathcal{L}^C and \mathcal{L}^E have different boundary conditions.

Using a single field solver ensures consistency of the fields in both codes



Correctness of the field is not ensured when Core and Edge solve for the field with different boundary conditions.

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What is EFFIS 2.0?

Workflow
Composition

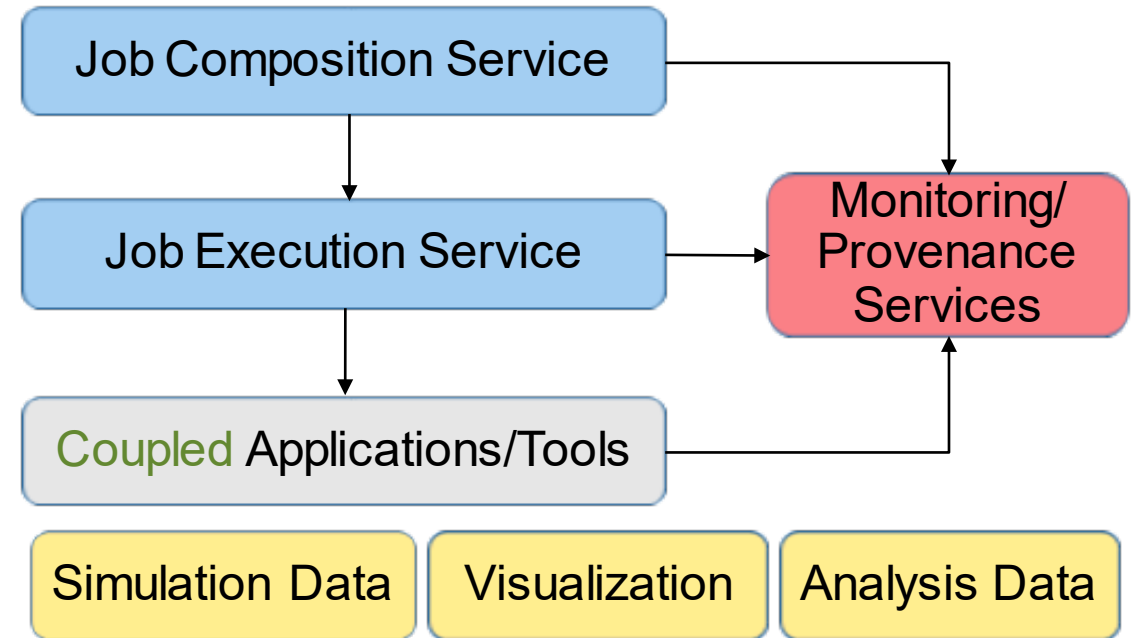
Communication

Monitoring/
Provenance

Toolkit

Output

- EFFIS 2.0 is a workflow coordinator for the WDM App
 - A collection of services to **compose**, launch, **monitor**, and **communicate** between coupled applications
 - Automates “easy” deployment on DOE systems
 - Facilitates “easy” integration to analysis and visualization tools, components, frameworks, etc.
 - Unique features: in-situ memory-based data movement, placement options (e.g. same node), wide-area network, automated visualization



Optimization of GENE, XGC and GEM for large-scale Summit

Scope and objectives

- Port and optimize WDMApp codes on Summit computer in preparation for exascale systems
- Leverage the ECP Co-Design and Software Technologies projects for portability and performance
- Scale WDMApp codes GENE, XGC, and GEM to 20% of Summit

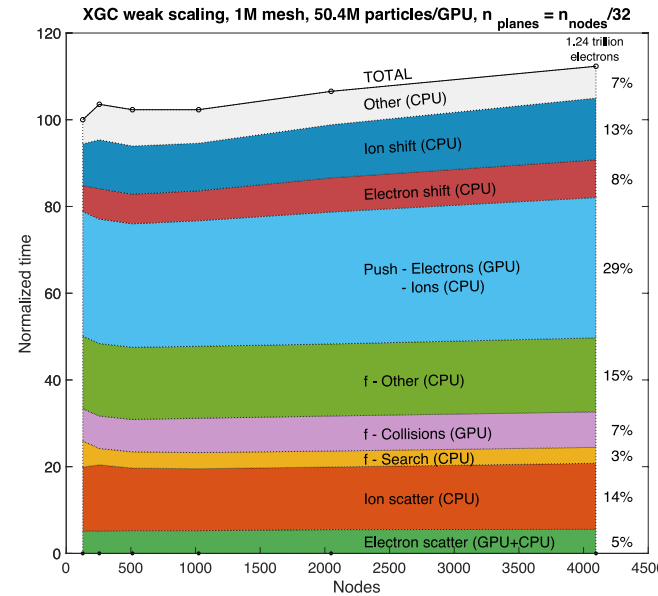
Impact

- Achieving high performance and scalability on a multi-GPU system is a critical requirement towards running WDMApp on Frontier and Aurora

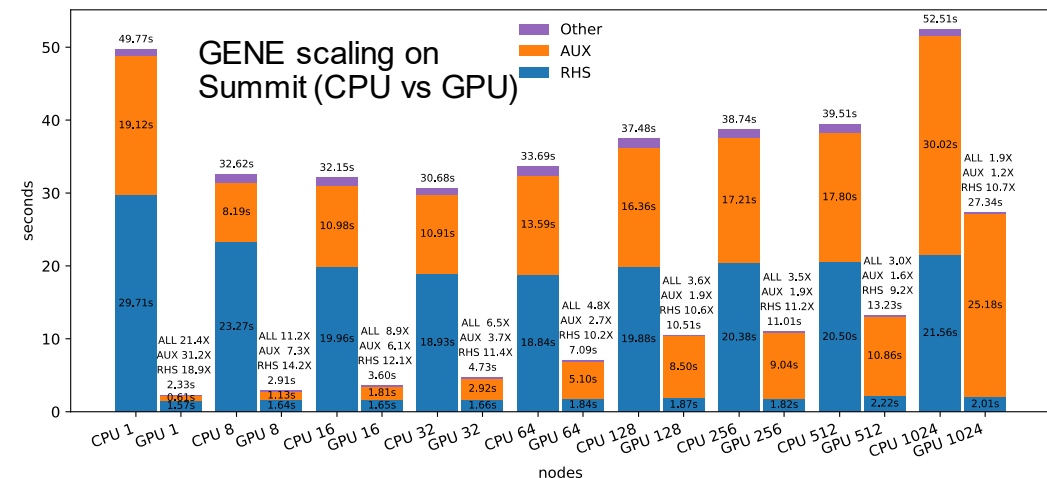
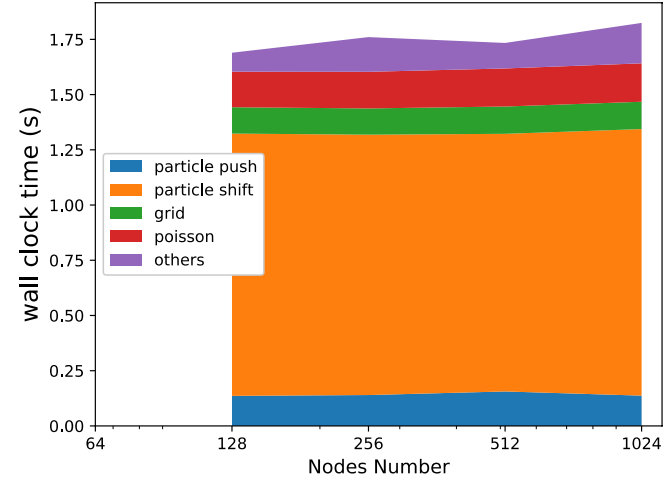
Project accomplishments

- Successful porting to GPU of all three codes used in the WDM application: XGC, GENE, and GEM
- Use of CoPA-developed “Cabana” library in XGC, leading to high portability without loss of performance or scalability
- All 3 codes successfully ran on 1,024+ nodes on SUMMIT

ECP WBS ADSE12-16 WDMApp
PI Amitava Bhattacharjee, PPPL
Members PPPL, ORNL, ANL, LBNL, UNH, UT-Austin, UC-Boulder



GEM particle scaling (fixed grid) on Summit



Conclusions

- WDMApp is a leading priority of the fusion community and will deliver a computational tool of unprecedented power and versatility.
- We have focused here on two primary goals: (1) Coupling of core gyrokinetic code (GENE and GEM) and edge gyrokinetic code (XGC), and performance of the coupled code with FOM > 50 (2) Development of a user-friendly extensible framework EFFIS 2.0 for code-coupling in WDMApp.
- The science is potentially transformational, and compute power will help realize Hawking's vision for fusion in the 21st century.

Thank you for your attention!
Questions ?