Exascale Computing and Whole Device Model for Fusion

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EXASCALE COMPUTING PROJECT

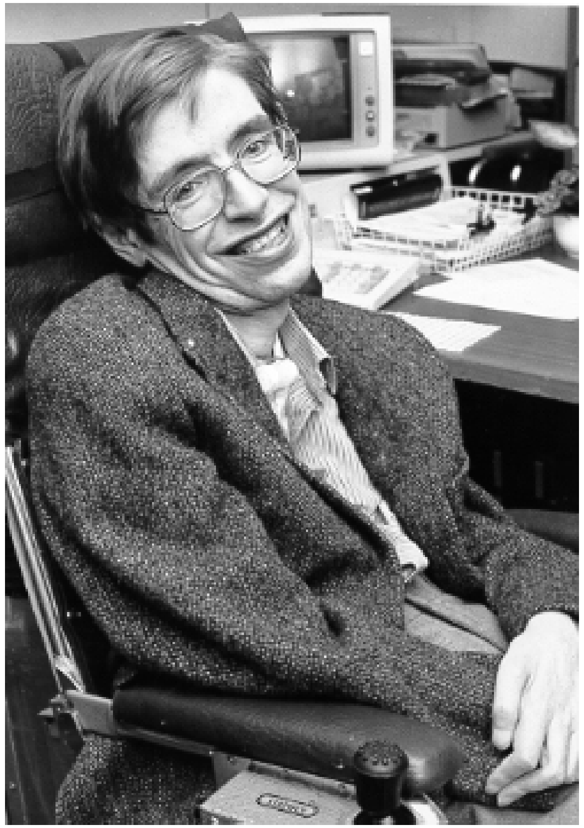
National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY | Office of Science

www.ExascaleProject.org

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

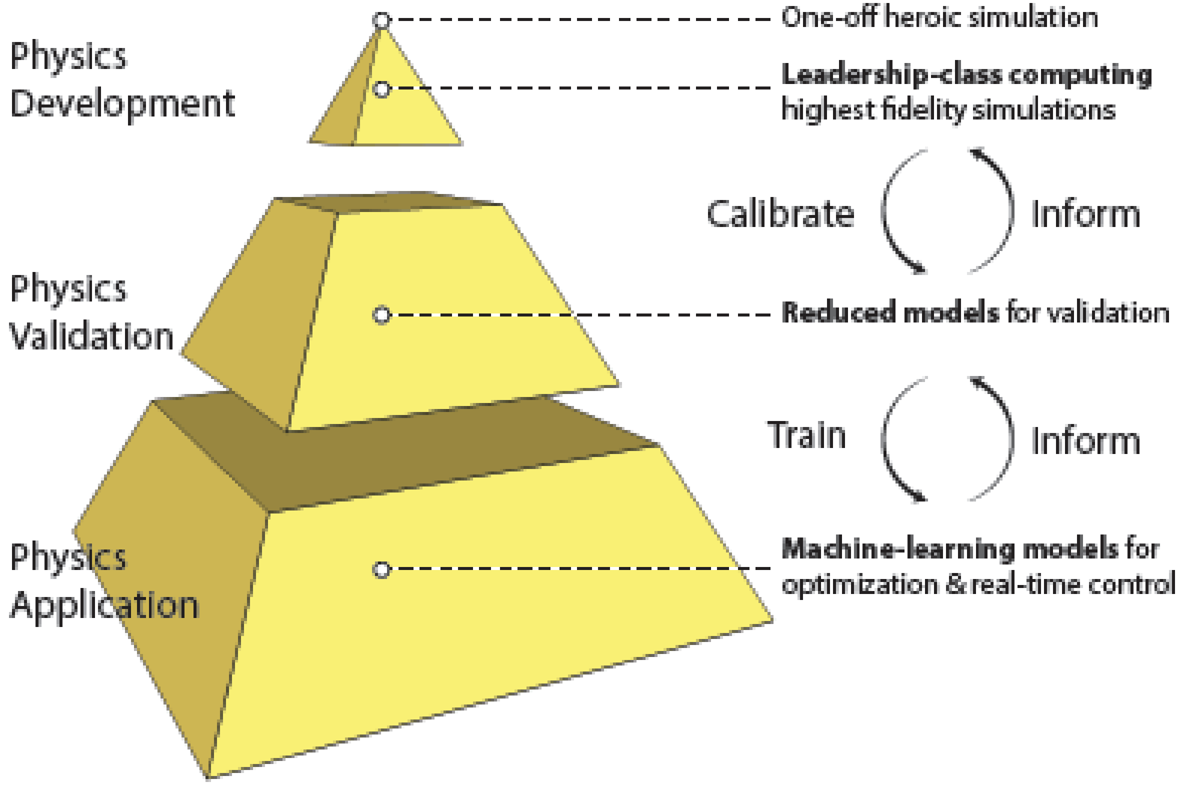


1942-2018

WDM hierarchy: High-fidelity to reduced models

Fidelity Hierarchy is CRITICAL

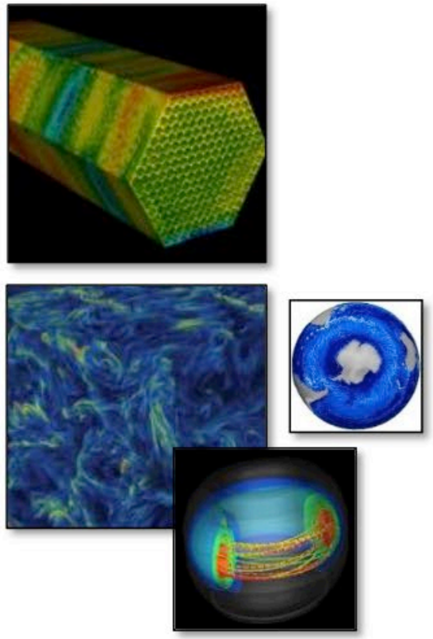
Range of models from leadership codes to REDUCED MODELS

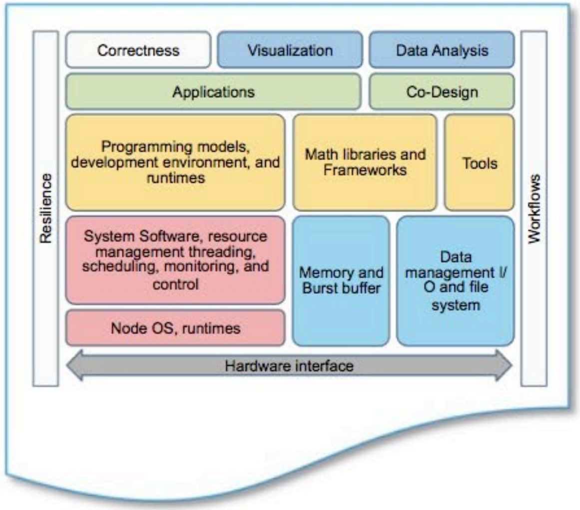


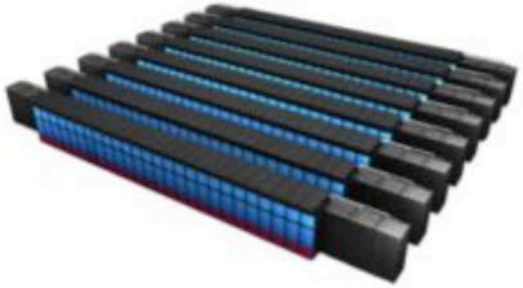
Courtesy: J. Candy

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

Application Development	Software Technology	Hardware Technology	Exascale Systems
Science and mission applications	Scalable software stack	Hardware technology elements	Integrated exascale supercomputers

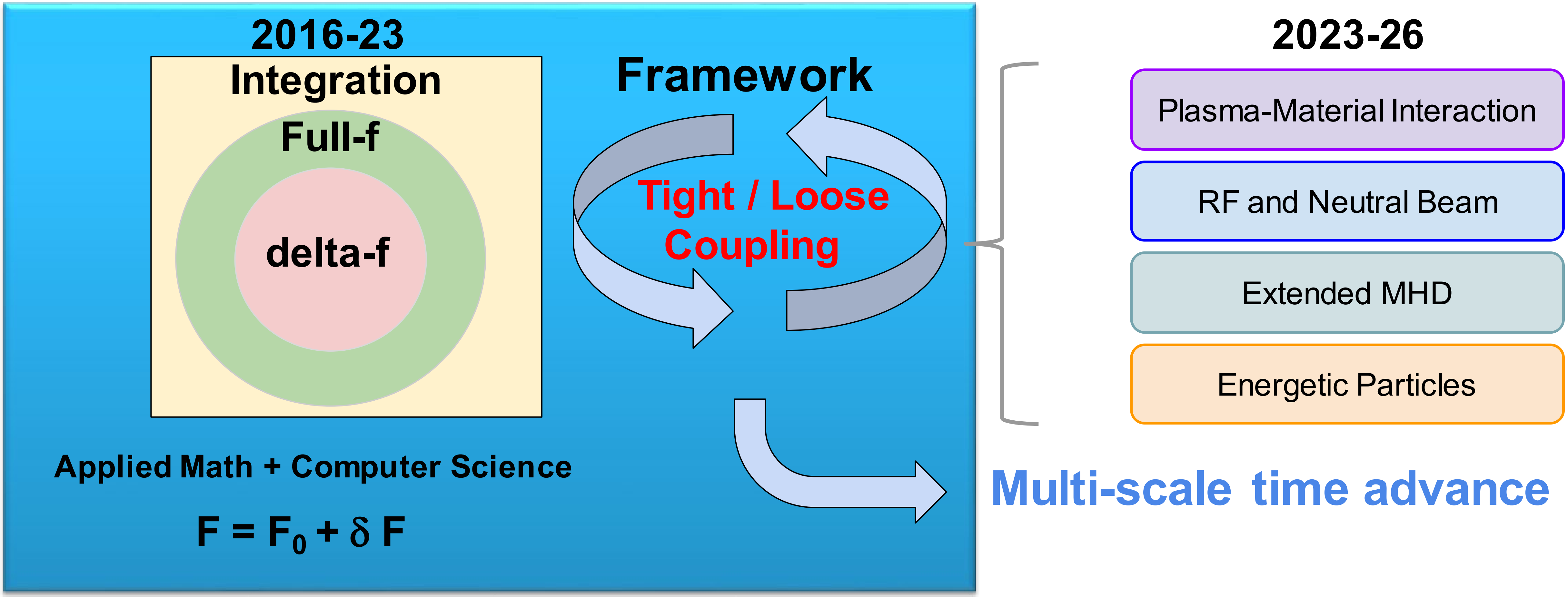






Exascale computers: 10^{18} floating-point operations per second (64-bit floating point precision)

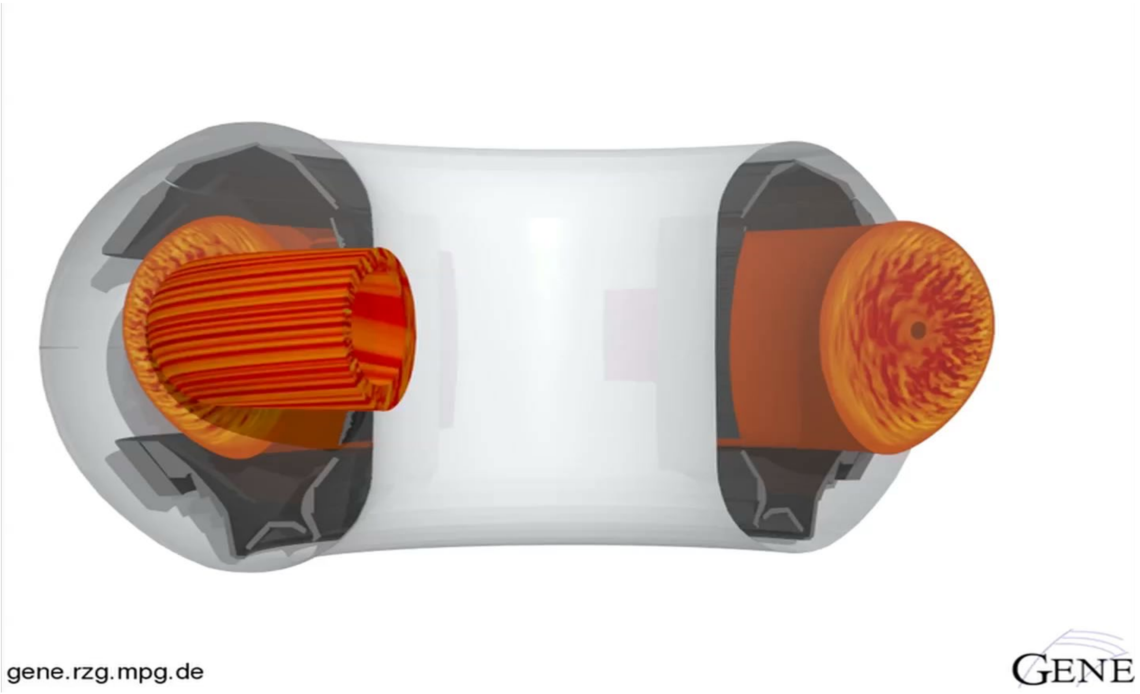
Vision: A High-Performant, First-Principles-Based Whole Device Model



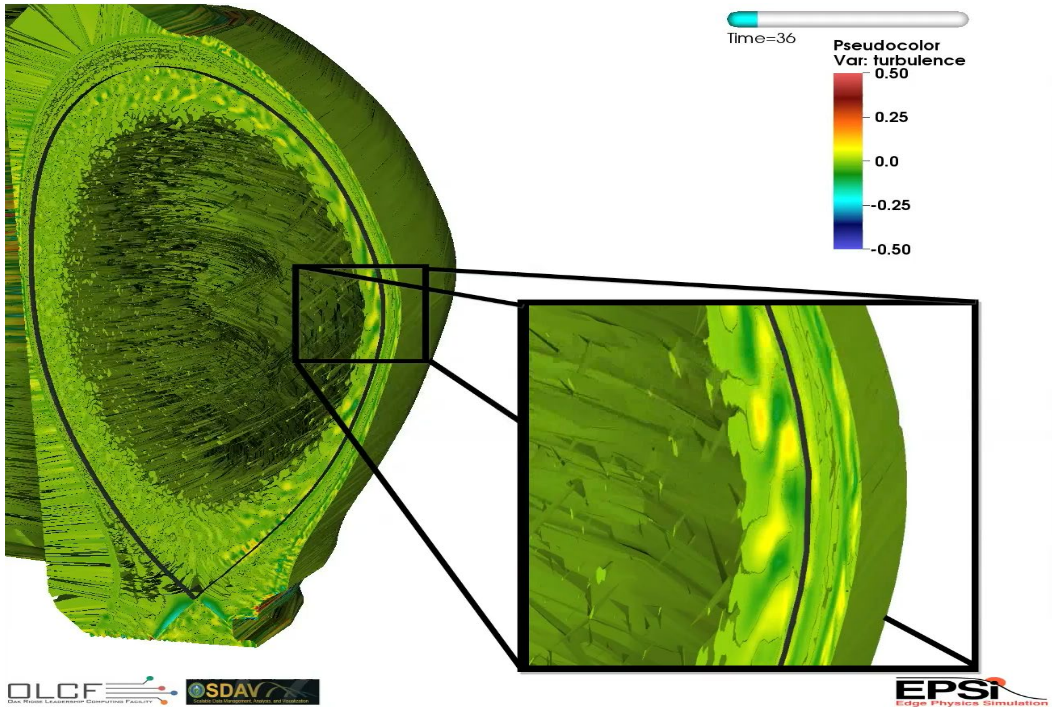
Coupling the core and edge: first in fusion history

The core evolves more slowly than the edge

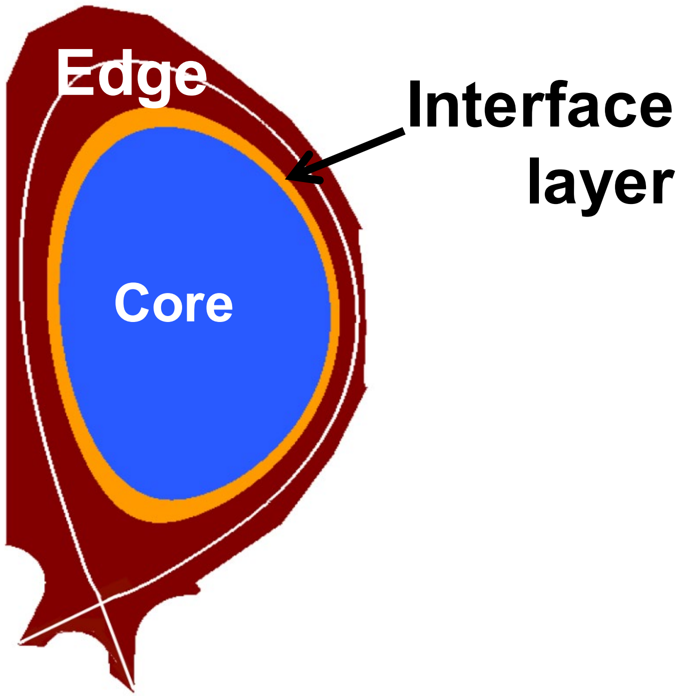
Core Turbulence from GENE



Edge Turbulence from XGC



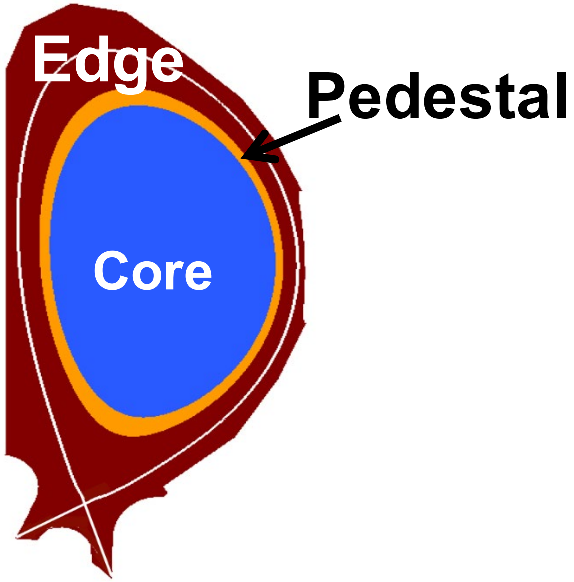
Principal WDMApp Goals



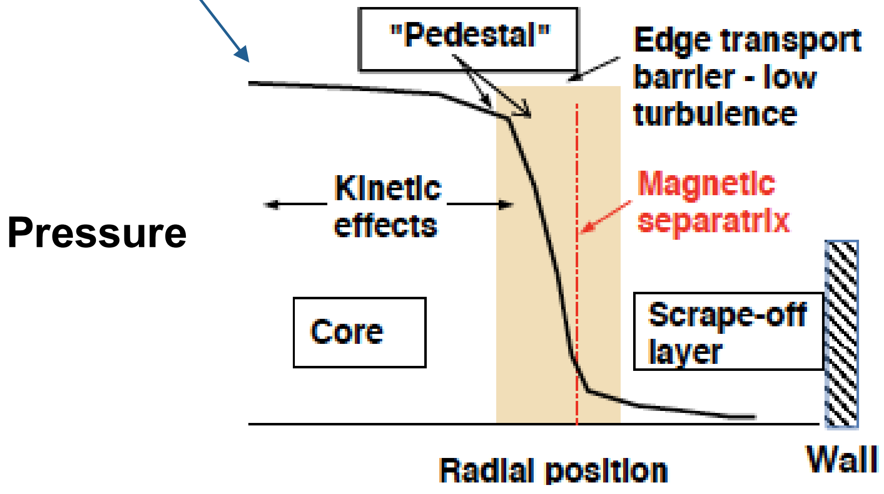
- Demonstration and assessment of WDM **gyrokinetic physics** on experimental transport time-scale in a challenge problem for pedestal formation
- **Figure of Merit (FOM) of >50** for coupled code on exascale platforms, accomplished through algorithmic advancement, performance engineering and hardware 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

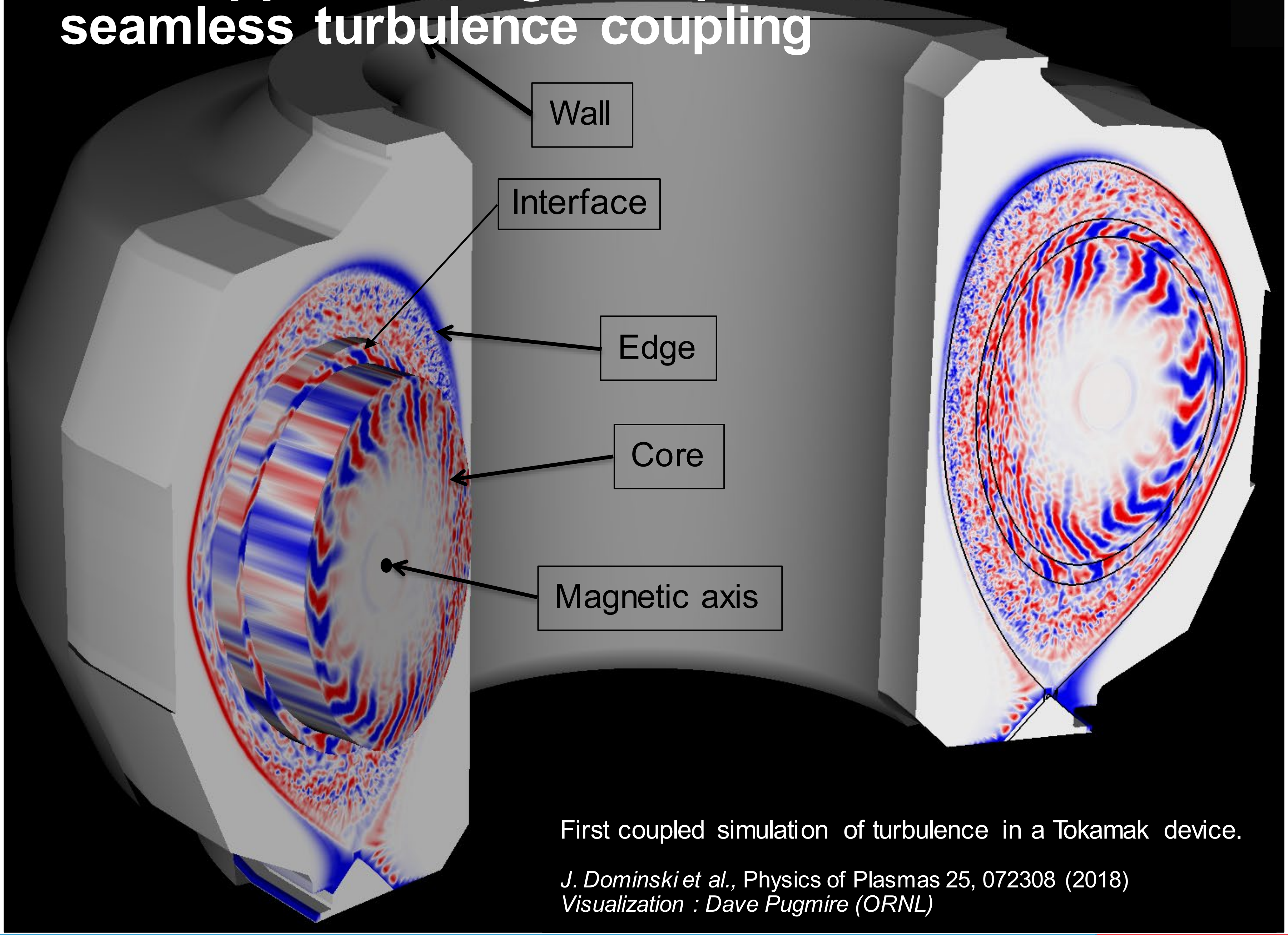
High-fidelity simulation of a whole-device burning plasma (specifically, ITER with full plasma current) operating in “high-mode” (H-mode), and prediction of the plasma pressure “pedestal” shape (height and width)



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



WDMApp Core-Edge Coupled Simulation shows seamless turbulence coupling



First coupled simulation of turbulence in a Tokamak device.

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

Developing core-edge coupling of technology

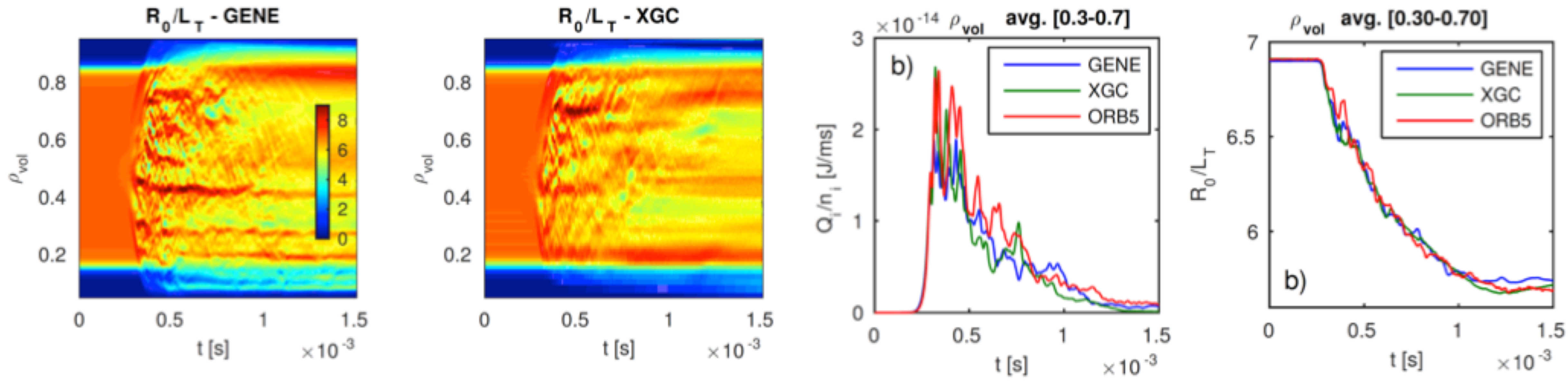
1. We first use XGC-XGC coupling to develop the technology

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.

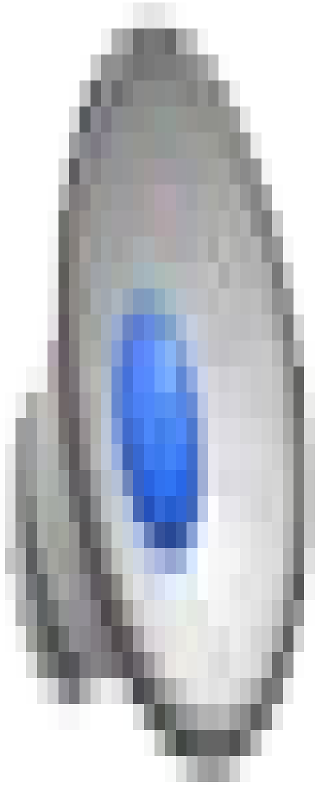
Cross-verification between GENE and XGC:
Non-linear ITG instability (J. Dominski, S. Ku, G. Merlo, C.S. Chang, F. Jenko, S. Parker)



Time-radius dynamics of the logarithmic gradient R_o/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

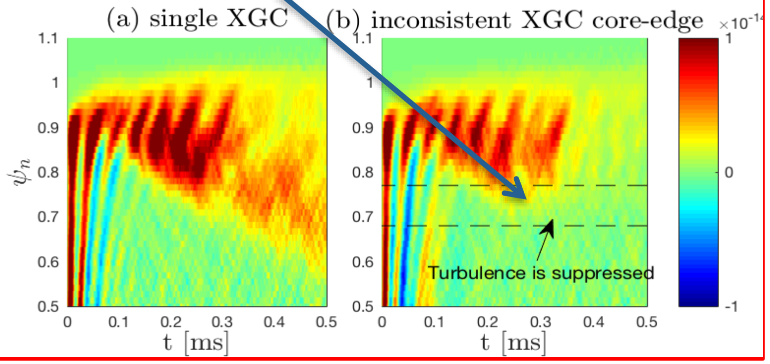
Implemented by J. Dominski, S.H. Ku, and C.S. Chang.

- 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

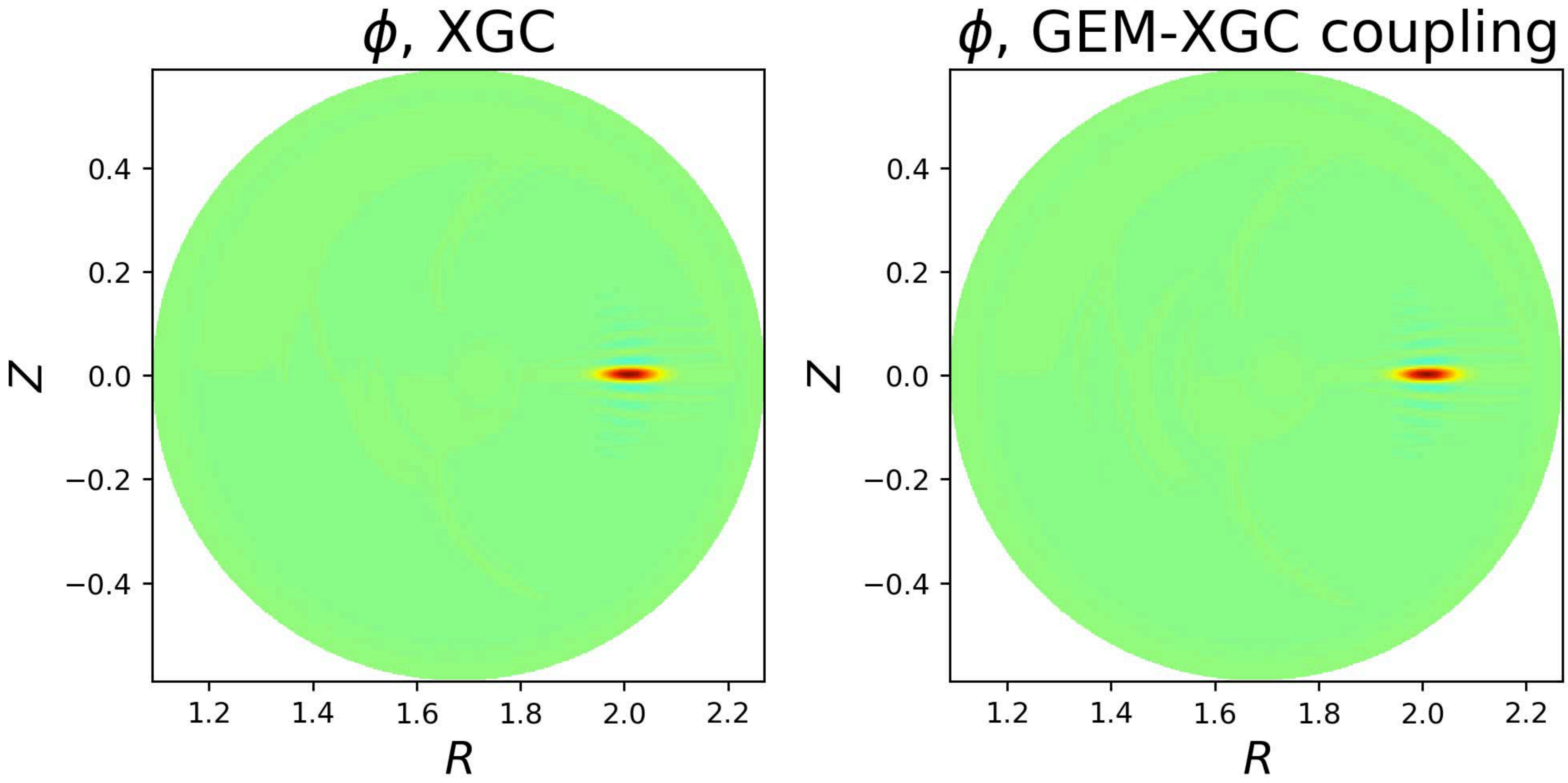
Difficulty was in avoiding turbulence suppression from nonlinear de-phasing between two codes.

Failed example

Ion heat flux, Qi

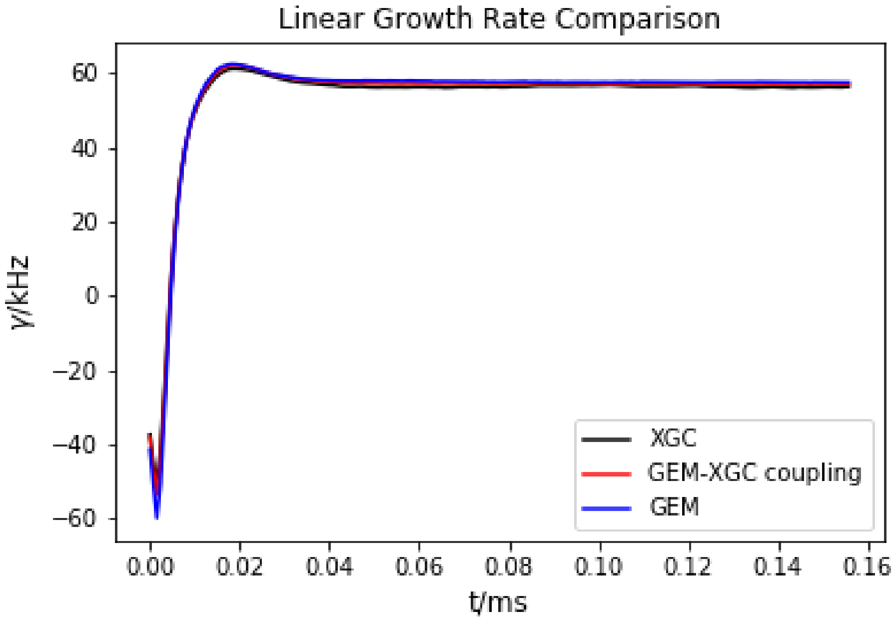


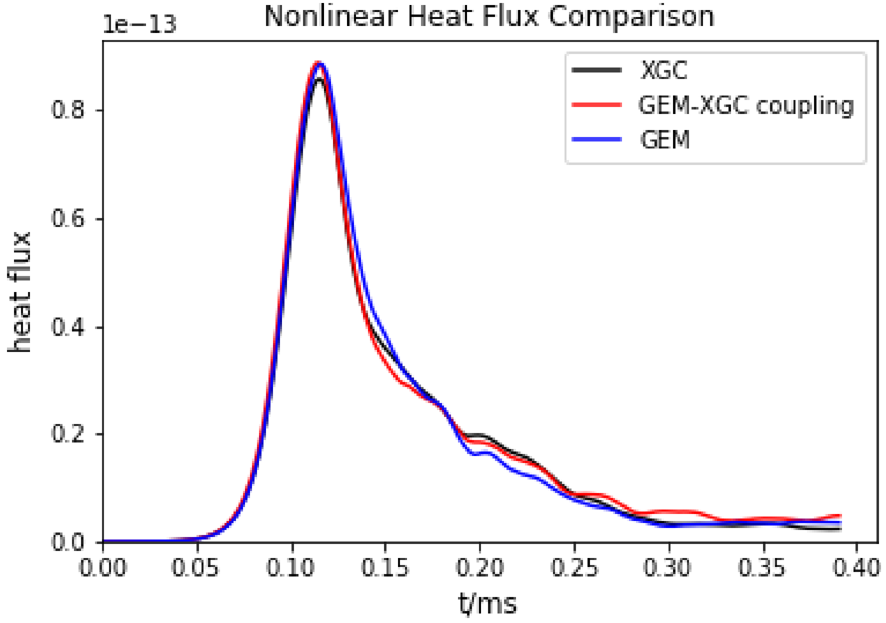
XGC – GEM coupling



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

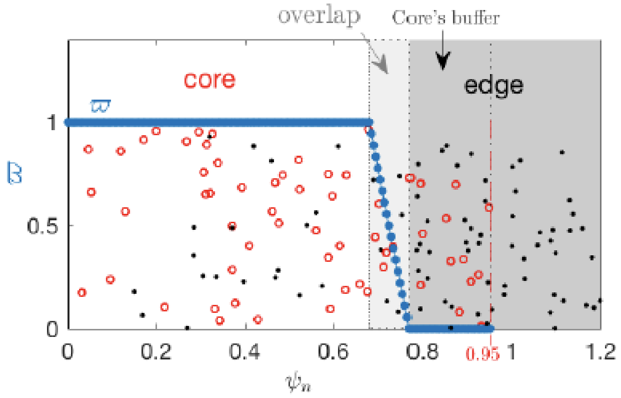
Spatial Core-Edge Coupling

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

$$\bar{n}[\delta\check{f}] = \int d\boldsymbol{X} dv_{\|} d\mu d\alpha\, \delta_{gc} \Big[\underbrace{\varpi(\boldsymbol{X})\delta f^{\mathrm{C}}}_{\text{local in core}} + \underbrace{(1-\varpi(\boldsymbol{X}))\delta f^{\mathrm{E}}}_{\text{local in edge}} \Big]$$
$$= \bar{n}[\varpi\delta f^{\mathrm{C}}] + \bar{n}[(1-\varpi)\delta f^{\mathrm{E}}].$$



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)]

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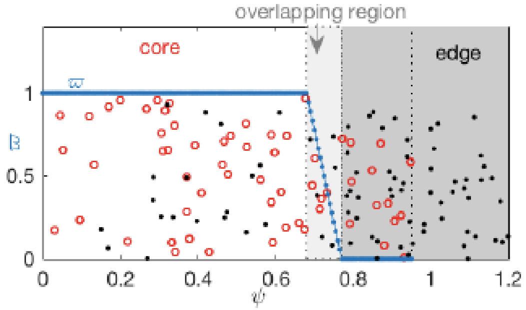
Question: Hallatschek

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.



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

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

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

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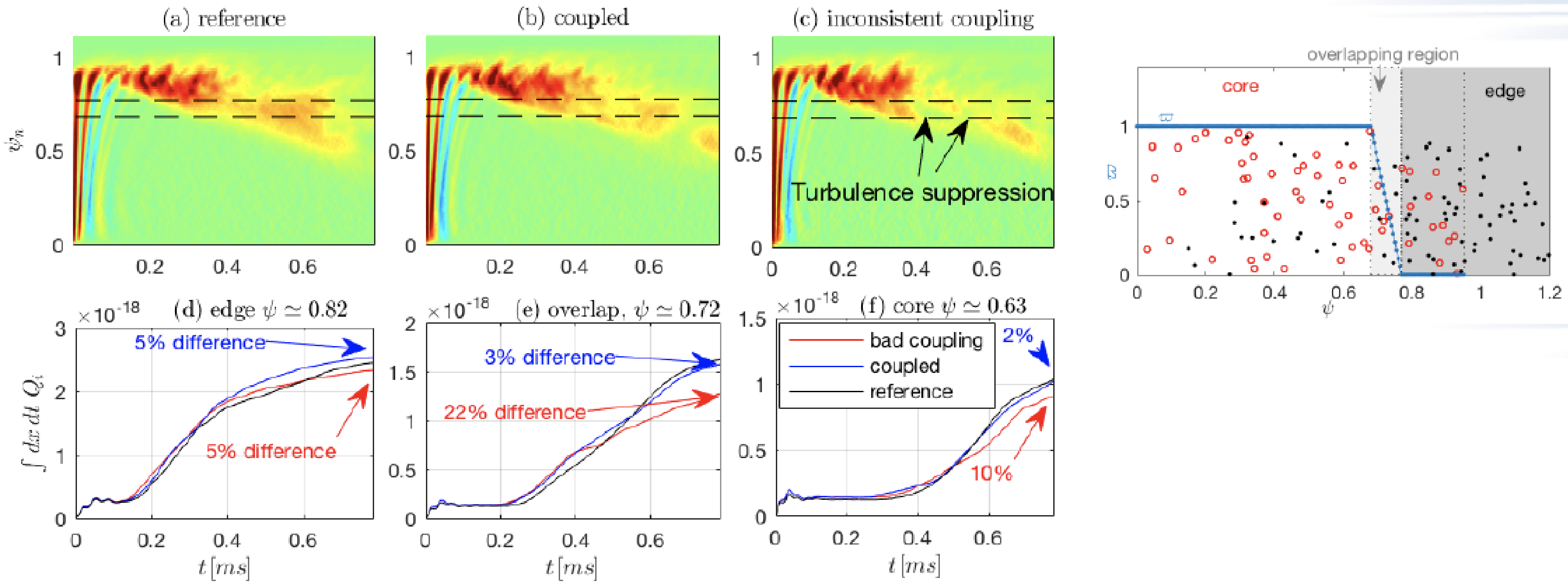
Using a single field solver ensures consistency of the fields in both codes



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

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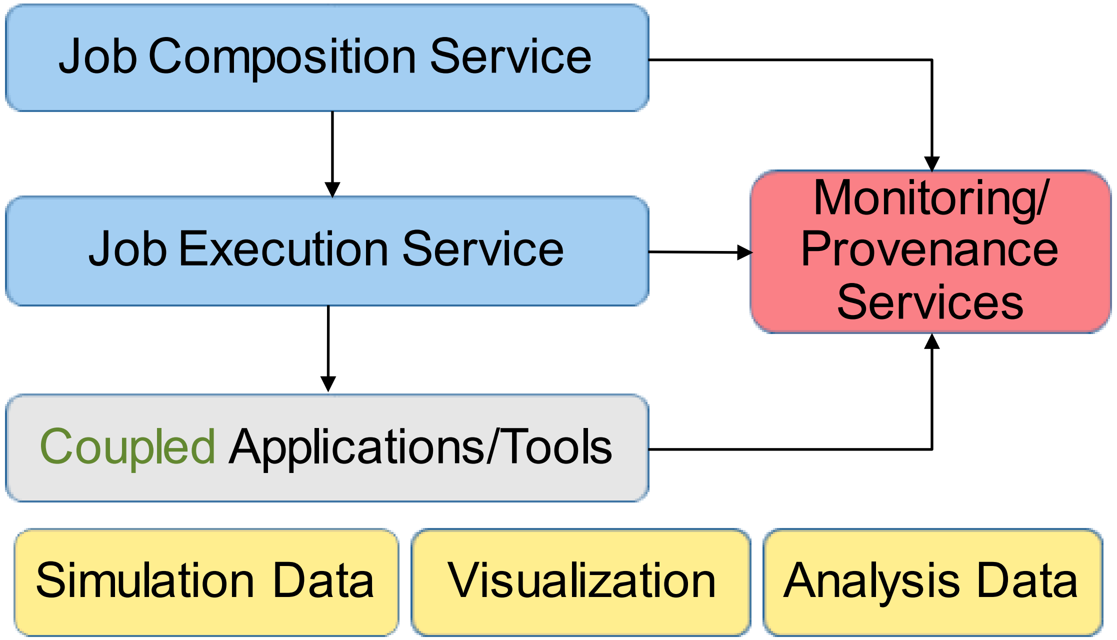
What is EFFIS 2.0?

- 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

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

Scope and objectives

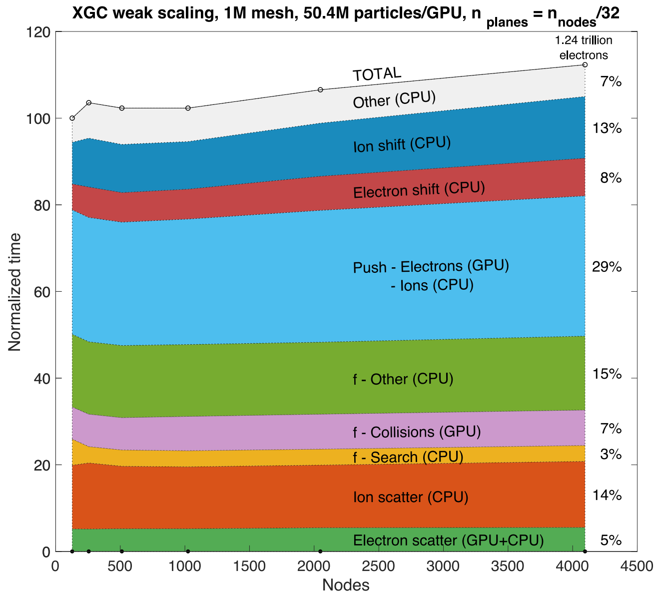
- Port and optimize WDMApp codes on Summit computer in preparation for exascale systems
- Leverage the ECP Co-Design and Software Technologies projects for portability and performance
- Scale WDMApp codes GENE, XGC, and GEM to 20% of Summit

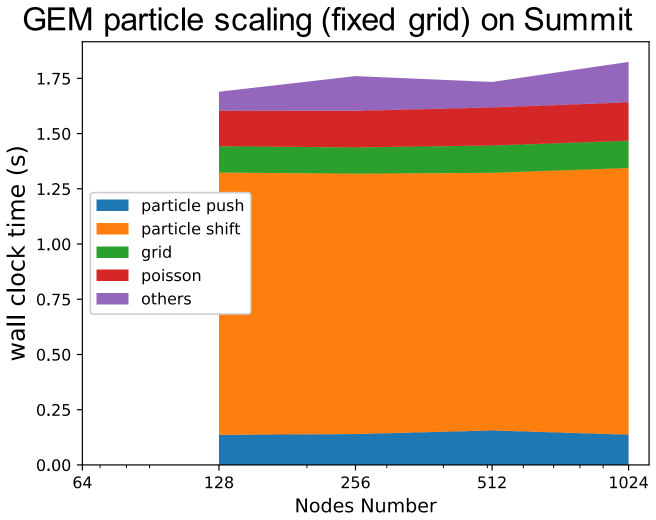
Impact

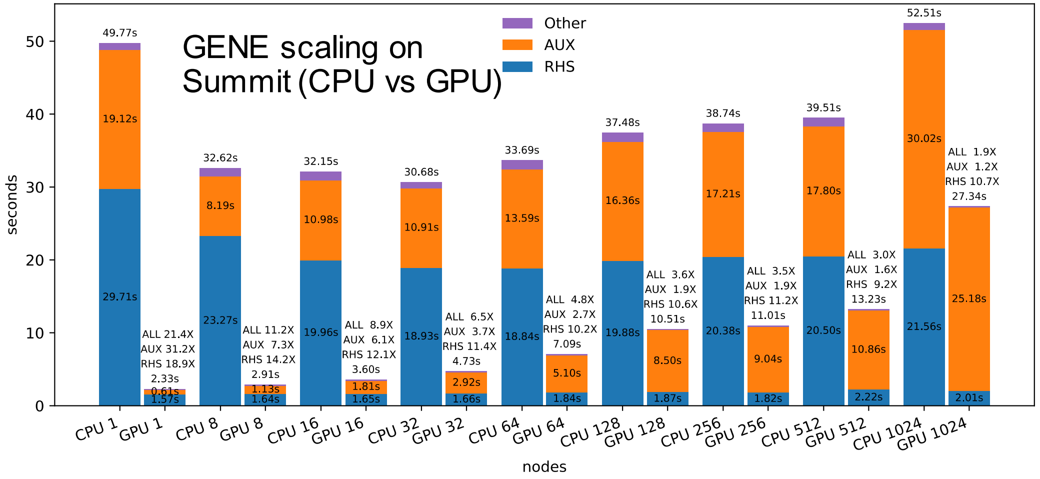
- Achieving high performance and scalability on a multi-GPU system is a critical requirement towards running WDMApp on Frontier and Aurora

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







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 ?