Partnership for Multiscale Gyrokinetic (MGK) Turbulence

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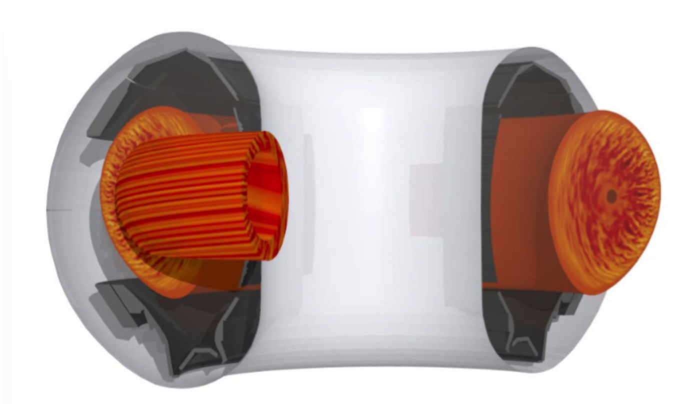
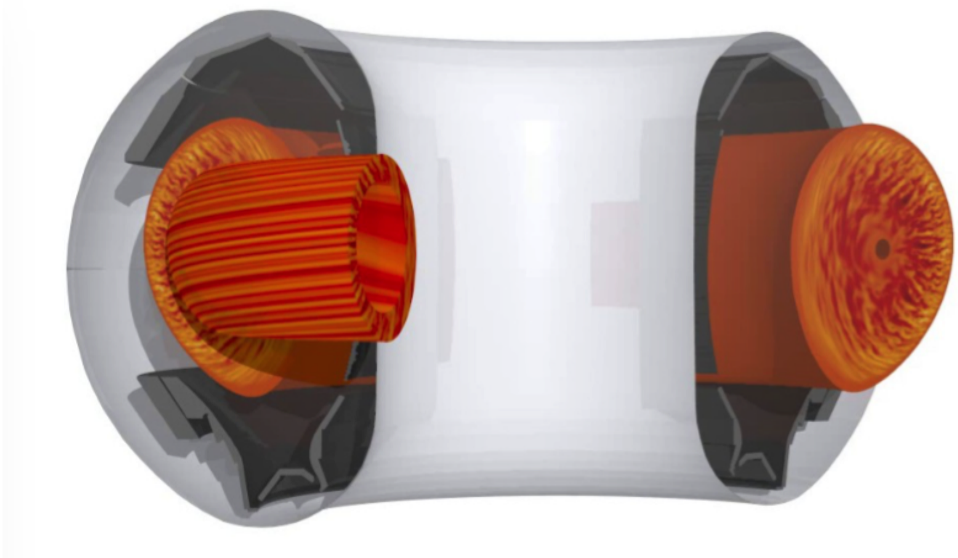


SciDAC MGK

mgkscidac.org

MGK Partnership (mgkscidac.org)

- Achieve profound scientific breakthroughs on ‘frontier’ multiscale turbulent transport problems
- Develop practical new methods to bring these problems within the scope of whole device modeling
- Ultimately: integrate with AToM framework



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Multiscale Gyrokinetic Turbulence

- Kinetic turbulence: evolve f(**x**,**v**,t)
  - Turbulence is multiscale in **all** dimensions
  - Time scales: Turbulence vs Transport
  - Spatial scales:
    - Equilbrium vs fluctuations
    - Ion vs Electron
  - Phase space (scales in velocity space)
    - Low vs high order moments (i.e. fluid vs kinetic)
  - MGK addresses multiscale issues in **all** dimensions
- Multiscale phenomena can be an opportunity and a challenge
  - Opportunity: exploit scale separation to simplify
  - Challenge: need to address multiple scales directly

Frontier Multiscale Turbulent Transport Problems

Exploit Multiscale

- Bridging the gap between turbulence and transport time scales for global turbulence [TANGO code]
- Ion-electron multiscale turbulence [GENE, Gkeyll codes]
    - Practical algorithms for fast/efficient cross scale coupling
- Hermite-Laguerre gyrokinetic code [GX code]: seamless transition between fluid and kinetic to optimize rigor-efficiency

Deal Directly with Multiscale

- Turbulence in transport barriers (H-mode pedestal, Internal transport barriers) [GENE, Gkeyll codes]
- Ion-electron multiscale turbulence [GENE, Gkeyll codes]
    - Full multiscale simulations in H-mode pedestal
- New kinetic algorithms [Gkeyll]

Tango: Turbulence + Transport

Goal: use first-principles gyrokinetic turbulence simulations to predict plasma behavior at long experimental timescales.

- *Problem:* Direct numerical simulation capturing both turbulence and confinement timescales is prohibitively computationally expensive, and could infrequently be performed

Turbulence time ~ 10 μs
Energy confinement time ~ 1 s

Vision: Multiscale method to exploit the timescale gap.

- Couple ***a transport solver*** with **global gyrokinetic simulation** for calculation of fluxes, e.g., using GENE
- *Challenge*: Need efficient methods and algorithms for coupling directly with global turbulence simulation $\frac{\partial n}{\partial t} + \frac{1}{V'}\frac{\partial}{\partial \psi}\left[V'\langle \mathbf{\Gamma}[n] \cdot \nabla \psi \rangle\right] = S_n$

Benefits: High-fidelity predictive turbulence + transport simulations. Can be a key component of a comprehensive whole-device model

- Transport at the confinement timescale, using best available gyrokinetic simulations as a high-cost, high-benefit alternative to computationally cheaper quasilinear transport models
- Nonlocal effects – e.g., internal transport barriers (ITBs)
- Enabling a new form of discovery science

Tango: Turbulence + Transport

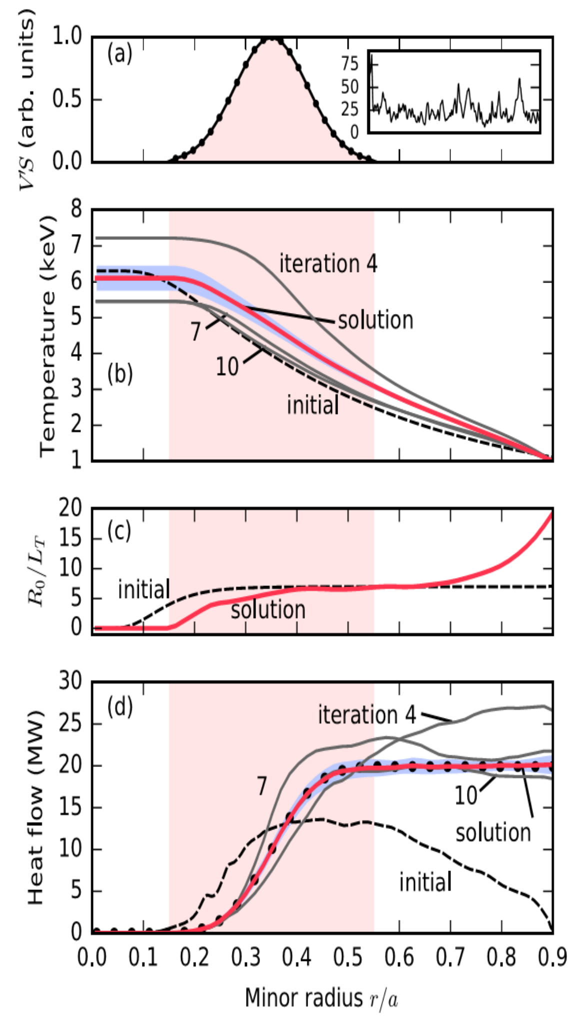
Tango:

- 1D transport code that implements method from [1] for coupling transport with global turbulence simulations
- Open source, in Python, available on GitHub
- Currently coupled to global GENE

Plan & Goals:

- Ratchet up to increasing physics fidelity – requires generalizations of the coupling method, handling multi-channel turbulent transport, etc.
    - Synergies with AToM possible
- **Simulate frontier physics, such as ITBs**
- **Demonstrate real-world value by enabling quantitative predictions for experiments**

Convergence to steady state temperature profile for a specified input heating power



References:

[1] A. Shestakov, R. Cohen, J. Crotinger, L. LoDestro, A. Tarditi, X. Xu, *J. Comp. Phys.* (2003)

[2] J. Parker, L. LoDestro, D. Told, G. Merlo, L. Ricketson, A. Campos, F. Jenko, J. Hittinger, *Nucl. Fusion* (2018).

[3] J. Parker, L. LoDestro, A. Campos, *plasma* (2018)

The Gyrokinetic GENE Code

Gyrokinetic Electromagnetic Numerical Experiment

(genecode.org; Jenko et al PoP 2000)

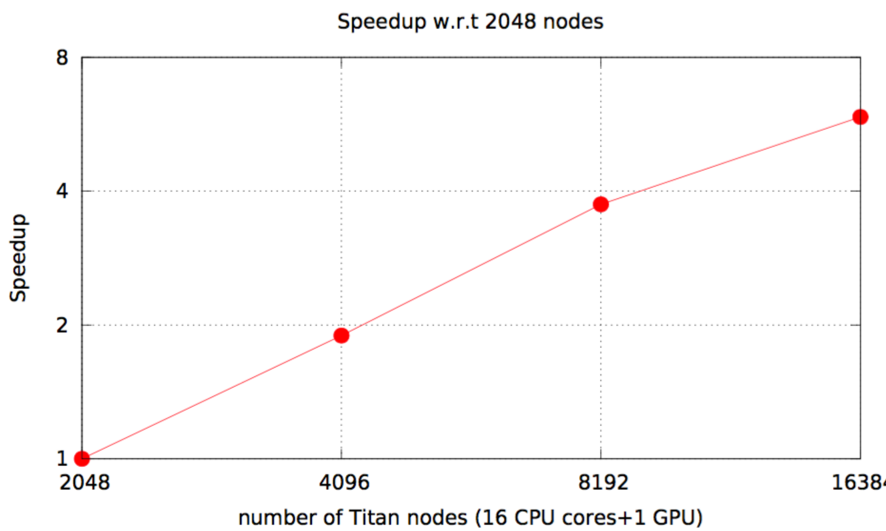
- Continuum approach to gyrokinetics (evolve distribution function on grid).
- Publicly available, world-wide user base from ~30 scientific institutions (US), ~100 worldwide
- Modes of operation:
  - delta-f & full-f (gradient-driven, flux-driven)
  - flux-tube & full-flux-surface & global
- Unique combination of various FDM, and spectral methods
- Extensive physics: kinetic electrons, electromagnetic effects, collisions, realistic MHD equilibria, electron-scale turbulence…
- Part of fusion whole device modeling ECP project

GENE on top-level HPC resources

PRACE

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

INCITE Award (2016)



Strong scaling of GENE on Titan (2k-16k nodes)

RAPIDS—Performance Tuning of GENE Code on the Intel KNL Architectures

- RAPIDS—Shan Hongzhang (LBL)
- Target Problem: P=2048 with 6D partition 1x2x8x16x1x8, 1 species

Current Progress

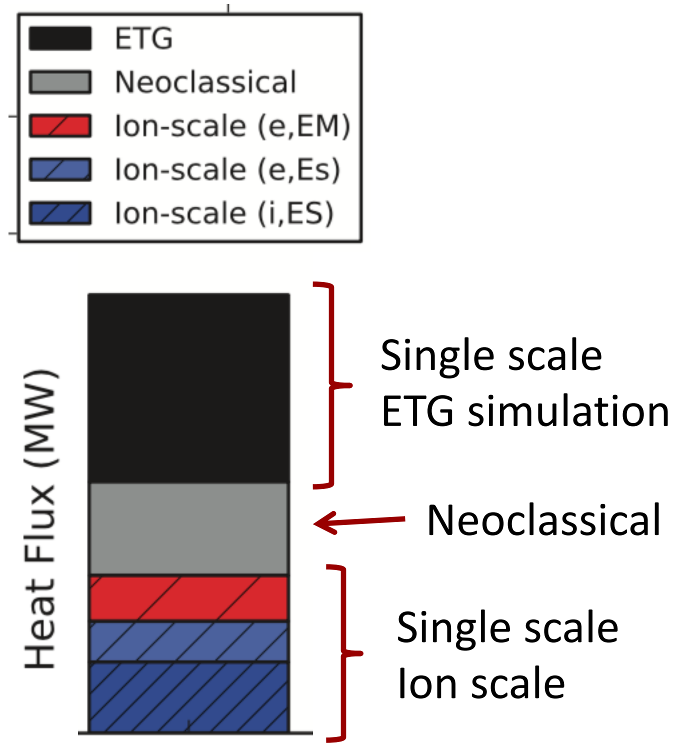
- Redesigned the timer so that its overhead can be ignored
- Profiled the code to identify important functions and loops
- Improved the communication performance about 15% by avoiding using the user defined MPI data types for non-contiguous data

Future Work

- Study the FFT performance, which consumes about 30% of the total time
- Rewrite some loops and data structure to improve vectorization
- Study the OpenMP performance effects

Pedestal Turbulence with GENE

- Recent breakthroughs in pedestal turbulence with GENE ([Hatch et al NF 2016, 2017; Kotschenreuther et al NF 2017])
- Goals:
  - UQ for pedestal turbulence:
    - Test errors/uncertainties in exp. input
    - Develop reduced models, surrogates
    - Compare against experimental observations
  - Ion-electron multiscale: substantial transport at ion scales and electron scales. As yet no tests of cross-scale coupling (likely very different than core multiscale).
  - Develop ability to evolve pedestal profiles, predict pedestal structure, model and predict ELM free regimes (coupling with TANGO)



What is the role of cross scale coupling?

Gkeyll Code: novel kinetic algorithms, multiple SciDACS & Applications

Novel version of Discontinuous Galerkin (DG) algorithm, conserves energy for Hamiltonian system even with upwind fluxes. High-order local algorithms reduce communication costs, helpful for Exascale. New modal version 30x faster than nodal version, uses sparseness of modal interactions.

Framework: Lua over C++, uses ADIOS, Eigen, MPI, …
In HBPS SciDAC, collaborating w. ORNL applied math group on algorithm studies.
Many opportunities for collaboration: improve IO scaling, performance tuning, GPU porting, …

3 Main Versions, used in 3 SciDACs:

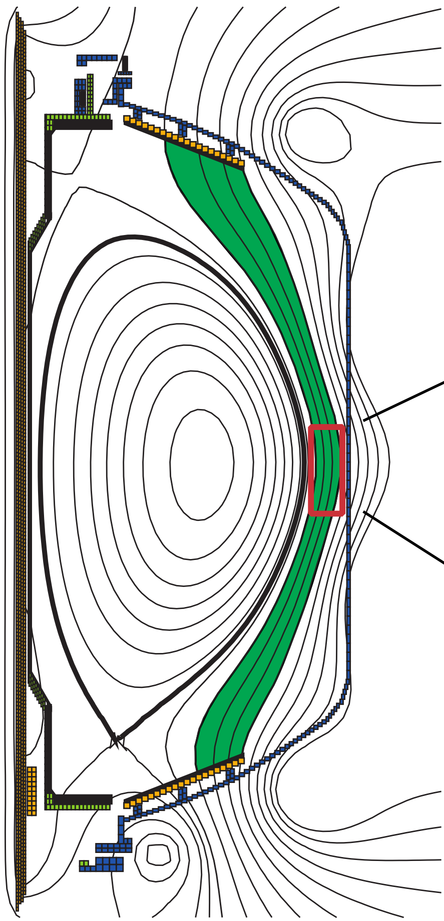
- Gyrokinetic DG version for edge turbulence in fusion,
  in MGK SciDAC project (D. Hatch, PI) for pedestal / multiscale work,
  in HBPS SciDAC project (C.S. Chang, PI) for scrape-off-layer turbulence work.

- Vlasov-Maxwell/Poisson DG version: solar wind turbulence (PU & U. Maryland), plasma-surface interactions in thrusters (AFOSR / Virginia Tech) & tokamak disruption SciDAC (LANL / Virginia Tech)

- Multi-moment multi-fluid (extended MHD) finite-volume version: reconnection (Princeton Center for Heliophysics), global magnetosphere simulations (UNH)

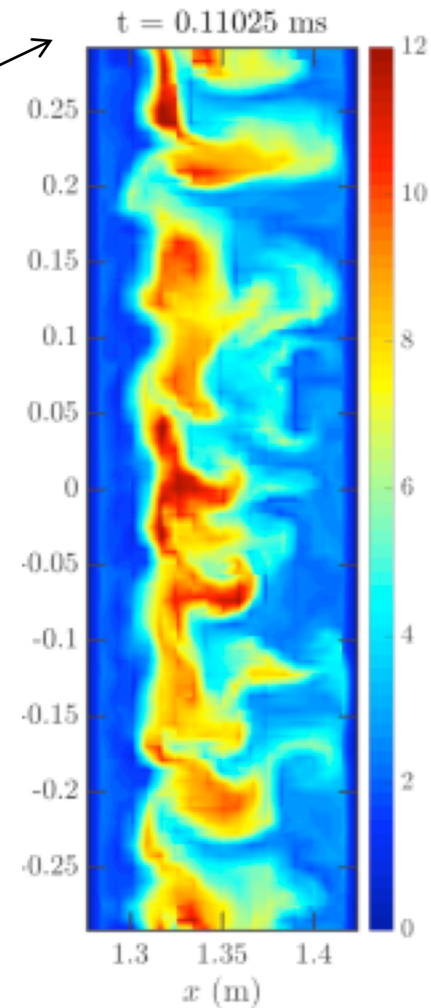
See poster by Ammar Hakim for more info.

Gkeyll: First Continuum 5D Gyrokinetic Simulations of Turbulence in SOL with sheath model boundary conditions



Edge region very difficult computationally.

XGC only code able to handle separatrix at present.



Various simplifications at present, such as helical model of SOL (toroidal + vertical B field).

E. Shi, A. Hakim, G. Hammett, et al. J. Plasma Physics (2017),
Q. Pan et al. Phys. Plasmas (2018), similar work in straight fields with GENE.

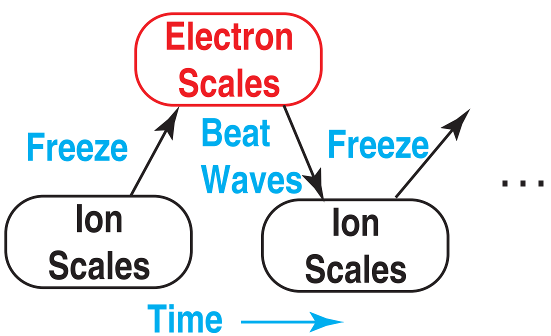
Practical Algorithms for Ion/Electron Multiscale Turbulence Interaction in Gyrokinetic Simulations

- Exploit factor ~60 scale separation in y-direction and time to significantly reduce computation time for turbulent transport with cross-scale coupling (MIT, PPPL, Texas, Maryland): $\Delta k_i \rho_i \sim \Delta k_e \rho_e \Rightarrow \Delta k_e \sim 60 \Delta k_i$ but presently $\Delta k_e \sim \Delta k_i$
- Non-local coupling between scales important in some scenarios

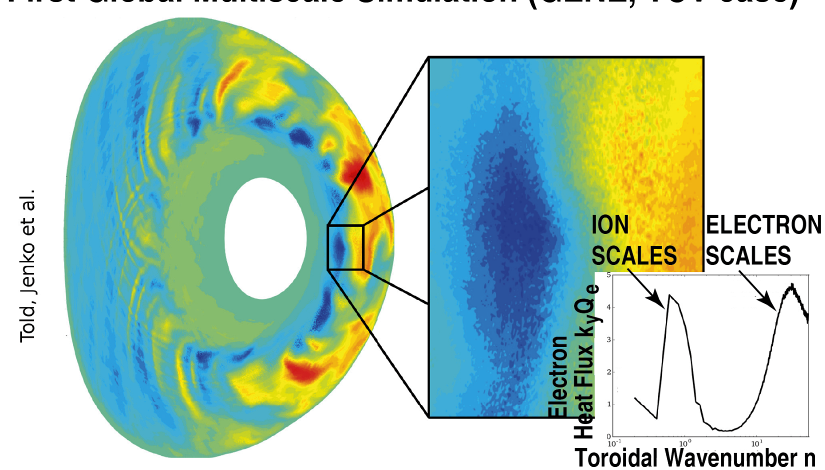
[Goerler (GENE), Maeyama(GKW), Howard(GYRO) heroic ~10's M hour gyrokinetic

Ion scales shear Electron scales	Electron scales damp ion scale zonal flows and beat into ion scales, increasing transport

- Algorithm: Save time by not using electron y-grid/timestep for ion scales



First Global Multiscale Simulation (GENE, TCV case)



- Use GKEYLL for initial 2d, one-field tests, then GENE; compare to full multiscale simulations

D. R. Ernst, G. W. Hammett et al.

MIT PSFC Plasma Science and Fusion Center

Formulated First Exact Linearized Landau Gyrokinetic Collision Operator in Conservative Form

- Conservative and symmetric structure enables a finite-volume or spectral discretization that preserves the conservation laws
  - Present model operators conserve globally, but are incorrect locally

- Initially implementing in the GENE code using finite-volume

- Future: Spectral methods with ~N scaling as well as Krylov-implicit methods; implementation in Gkeyll edge gyrokinetic code

$$C_{ab}^{\mathrm{gk}}\left(h_a, f_{b0}; f_{a0}, h_b\right) = -\nabla \cdot \underline{J}_{ab}$$ (Including FLR terms)

$$\underline{J}_{ab} \equiv \frac{\ln\Lambda}{8\pi}\frac{e_a^2 e_b^2}{\epsilon_0^2 m_a}\int 2\pi d^2 v' \left(\frac{h_a}{m_b}\underline{\underline{I}}_E^T \cdot \nabla_{v'} f'_{b0} - \frac{f'_{b0}}{m_a}\underline{\underline{I}}_D^T \cdot \nabla_v h_a + \frac{f_{a0}}{m_b}\underline{\underline{I}}_E^F \cdot \nabla_{v'} h'_b - \frac{h'_b}{m_a}\underline{\underline{I}}_D^F \cdot \nabla_v f_{a0}\right)$$

$$\underline{\underline{I}}_{E,D}^{F,T} = \int \frac{d\phi}{2\pi}\int \frac{d\phi'}{2\pi}\, g_1(\phi)\, g_2\left(\phi'\right)\, g_3\left(k\rho' \sin\phi' - k\rho\sin\phi\right)\left(\frac{\underline{\underline{I}}u^2 - \underline{u}\,\underline{u}}{u^3}\right)$$

$$\underline{u} = \underline{v} - \underline{v}'$$

$$g_j\left(x\right) \in \{1, \sin x, \cos x\}$$

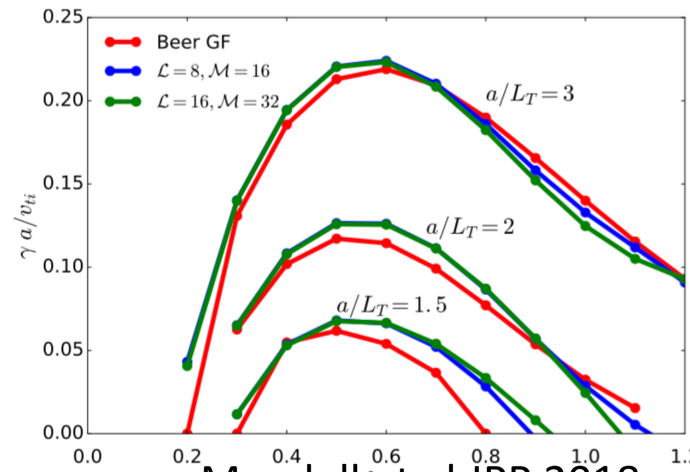
$\underline{\underline{I}}_{E,D}^{F,T}$ Gyrokinetic tensors for test-particle (field-particle) drag and diffusion coefficients

Q. Pan, D. R. Ernst

MIT PSFC Plasma Science and Fusion Center

GX code: Fluid vs Kinetic—why not both?

- GX code (Dorland et al)
  - Laguerre / Hermite in velocity space
  - Can use intelligent closures and be gyrofluid when applicable
  - Alternatively can keep lots of moments and be fully gyrokinetic
  - Status [Mandell, Dorland, Landreman, JPP 2018]:
    - Collision operator has been implemented
    - Linear closures tested / demonstrated
    - Extensive benchmarks of linear physics



Mandell et al JPP 2018

- Goals:
  - Seamless transition between fluid and kinetic descriptions depending on physical regime, desired speed / accuracy
  - Efficiently explore broad parameter space for optimization

Multi-fidelity database for UQ, V&V, ML

- Integrate MGK codes with OMFIT
  - Initial targets GENE (underway—Ernst), TANGO
  - Eventually Gkeyll and GX

- Develop database
  - Data groomed for integrated advanced data analytics (e.g. UQ, V&V, ML)
  - Experimental data curation (e.g. MDSplus, SQL)
  - Multifidelity simulation data (ranging from quasilinear to full global GK)
  - Develop UQ and ML algorithms for data mining
  - Integrate with AToM and related European initiatives (e.g. Minerva)
  - Initial efforts related to transport but could potentially be generalized to encompass phenomena of interest for other SciDAC areas (disruptions, etc)

- Goal:
  - Make multiple tools accessible within WDM framework
  - Use UQ /ML to identify tool that is most rigorous/efficient/predictive/fault tolerant, etc. for a given scenario

Inter-SciDAC Integration

- Connections with ATOM+OMFIT:
  - GENE+OMFIT integration underway (Ernst)
  - Using OMFIT to analyze our recent DIII-D experiments for IAEA 2018 oral: Profile fitting, Kinetic EFITs, TRANSP, Edge Stability Analysis
  - Future work?
    - Tango integration
    - ATOM codes (NEO, TGLF) integrated into Tango
    - Coordination of use cases (discussion with C. Holland)
  - Goal: all MGK codes/tools fully integrated and accessible within a whole device modeling framework
- Connections with HBPS
  - GENE benchmarking with XGC and GEM
  - Gkeyll development for scrape off layer
- Open to other connections where useful

Interaction with SciDAC Institutes

- Initiated collaborations with institutes
  - RAPIDS:
    - Profiling and optimization of GENE for Cori (KNL)
  - FASTMath
    - Initial contact about
      - Implicit solvers for collision operators
      - Multiscale algorithms

- Prospective topics for institute collaboration
  - (Artificially) Intelligent gyrofluid closures
    - Use machine learning to train fluid closures from kinetic simulations
    - Starting with simple toy problem
    - Eventual application to GX code
  - Gkeyll:
    - Improve scalability of IO—issues beyond a few thousand cores. Want to discuss with ADIOS group.
    - Help with performance tuning.
    - Porting to GPU
    - Post-processing, visualization, in-situ analysis