The Advanced Tokamak Modeling Environment (AToM) for Fusion Plasmas

Christopher Holland
University of California, San Diego

on behalf of the AToM team
http://scidac.github.io/atom/index.html

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AToM is 1 of 9 SciDAC-4 partnerships working to address modeling needs of US MFE program

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  assemblies of physics components that provide a sufficiently comprehensive integrated simulation of the plasma
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  - take a *bottoms-up, collaborative* approach that focuses on
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  - In practice, this means developing flexible software environment and workflows to couple existing and in-development physics components
AToM’s scope and vision extends from current-day devices to future reactor facilities

Present-day experiments
- Validate existing WDM capabilities
- Identify modeling gaps
- Drive new development

Support ITER
- Test WDM capabilities in burning plasma conditions
- Optimize ITER operation scenarios

Future reactor design
- Examine how to best optimize devices with varying goals and missions
Current AToM modeling capability enables coupled core-edge-SOL (CESOL) profile predictions

- **Future research directions:**
  - Self-consistent impurity transport from wall to magnetic axis
  - Implementing validated theory-based scrape-off layer (SOL) transport models

J.M. Park *et al*, 2018 IAEA FEC
AToM supports flexible workflows based on coupling of multiple physics components

- CESOL prediction requires coupling 15 physics components, executed on NERSC Edison Cray XC30 machine
AToM couples IPS and OMFIT computing frameworks and effectively exploits their synergy.
AToM modeling capabilities ready to support ITER research needs

- **Example**: modeling an ITER steady-state hybrid scenario

- AToM’s OMFIT framework includes full support for ITER IMAS data model
  - Enables access to ITER reference scenarios

- **Future work**: apply AToM capabilities to key ITER startup questions (e.g. H/He, half field/current operations)

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C. C. Petty *et al.*, Nucl. Fusion 2017
OMFIT STEP module supports discharge design and optimization for current and future machines

Predicted ITER steady-state $Q \geq 5$ scenario with day-1 heating

(J. McClenaghan et al, 2018 IAEA FEC)
AToM workflows will provide practical tools to design and optimize future reactors

• Combine efficient, validated tools with HPC resources to explore parameter space and optimize

• Example: AToM tools used to identify target operating scenarios for compact advanced tokamak DEMO (C-AT DEMO)

(R. J. Buttery et al, 2018 IAEA FEC)
Practical integrated studies require hierarchy of fast, efficient, and accurate physics components

Leadership-class computing

- highest fidelity simulations

Calibrate

Reduced models for validation

Train

Machine-learning models for optimization & real-time control

Inform

One-off heroic simulation
Core transport components provide template for future physics component development

- Nonlinear gyrokinetic simulations yield highest fidelity transport predictions but require $10^3 - 10^7$ core-hours to simulate small fraction of plasma volume & duration

Simulated $T_e$ fluctuations for a DIII-D discharge

C. Holland et al., Nucl. Fusion 2017
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- …but require **20+ million core-hours** to simulate a small fraction of plasma volume for a few milliseconds on current computing platforms

Simulated $T_e$ fluctuations for a DIII-D discharge

C. Holland *et al.*, Nucl. Fusion 2017
Core transport components provide template for future physics component development

- WDM predictions effectively require hundreds or more of such simulations for convergence
  - not currently practical

- Resolve bottleneck via reduced models that combine physics understanding and high-fidelity simulation results to make equivalent predictions in core-seconds

G. M. Staebler et al, Nucl. Fusion 2017
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- Improving and expanding reduced model capabilities requires significant increases in high-fidelity simulations
  - More parameters at higher resolution

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• Recent optimization work by AToM team members suggests a 10x increase in high-fidelity code performance on next-generation exascale platforms is possible

• Enables scope and scale of new high-fidelity simulations to improve our reduced models and thereby our practical predictive modeling capabilities
AToM working to deliver practical, high-fidelity whole-device modeling capabilities

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  – Improving reduced model components for areas such as core and edge transport
    • Bring “big data” and machine learning tools to bear here in addition to traditional approaches
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  - Development of a validation and future scenario use case database to track model development, coordinate with other SciDAC-4 centers
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• Longer term goal: partnering with other SciDAC centers to integrate and improve both high-fidelity and reduced model components for:
  – RF heating & current drive (PI: P. Bonoli)
  – energetic particle transport (PI: Z. Lin)
  – plasma edge & scrape-off layer physics (PI: C. S. Chang)
  – plasma-material interactions (PI: B. Wirth)
  – disruptions (PI: S. Jardin)
  – (PI: X. Tang)
  – runaway electrons (PI: D. Brennan)
Backups
OMFIT- One Modeling Framework for Integrated Tasks

http://gafusion.github.io/OMFIT-source/
IPS - Integrated Plasma Simulator

- Python-based HPC component framework
- Components are python-wrapped binaries
- Framework runs in a single batch allocation, manages resources for components
- Components launch task on compute nodes using standard system mechanisms
- PlasmaState holds primary data for exchange
- Reader-makes-right model
AToM has established a reliable infrastructure to generate machine-learning based reduced models.
Neural-net versions of TGLF and EPED achieve significant speed-up while maintain good fidelity

EPED1-NN trained on database of 20,000 EPED1 runs for DIII-D, KSTAR, JET, ITER, CFETR parameters (10⁹ speedup)

TGLF-NN trained (with TENSORFLOW) on database of 500,000 cases from multi-machine database (10⁵ speedup)

O. Meneghini et al, Nucl. Fusion 2017