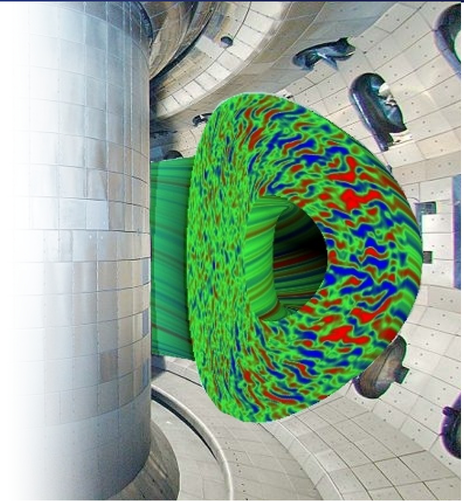
GA Theory Advanced Computing



by
GA Theory Group

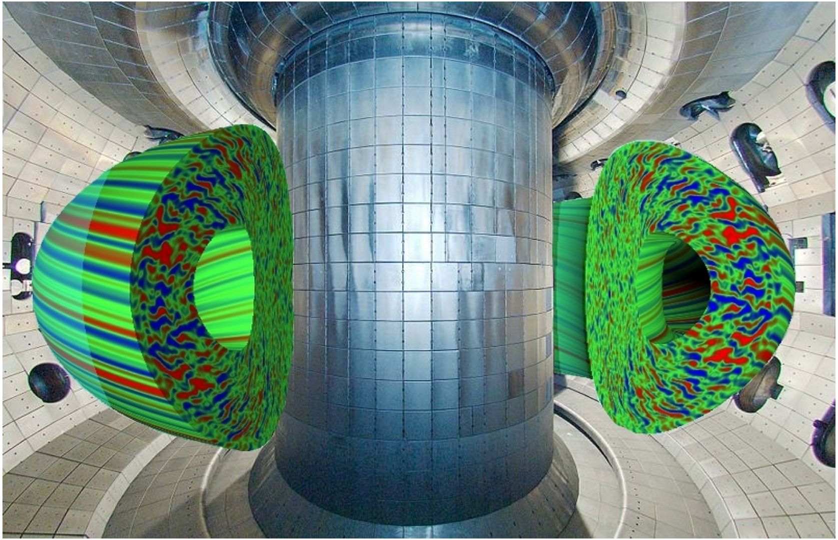
General Atomics, San Diego, CA

Working document

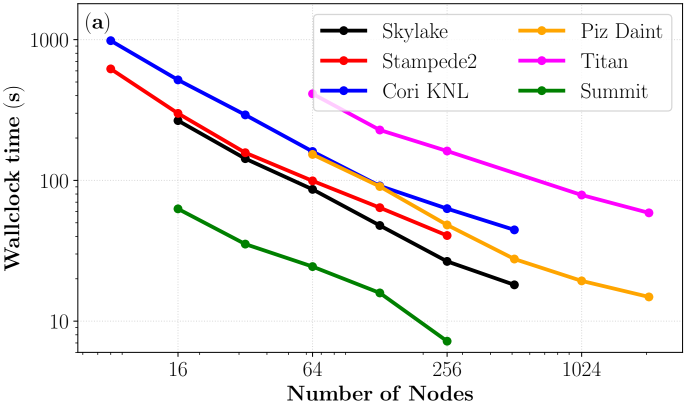
GA Theory Group: long history of HPC leadership

- Founded **San Diego Supercomputing Center** (1985)
- Strong connection to **DOE SciDAC program**
  - ATоM, CTTS, ISEP, PSI2, ESL, SCREAM
  - Various connections and collaborations with DOE ASCR scientists
- Winner of numerous HPC awards:
  - **INCITE (DOE), ALCC (DOE), XSEDE (NSF)**
  - Currently have **ALCC awards on OLCF Summit**
  - HPCWire feature articles (GYRO 2006, GYRO 2018)
  - Recent winner **2021 INCITE** (450M Summit hours)

GYRO/CGYRO: 20 years of gyrokinetic leadership at GA



Performance on Leadership Systems (US and Europe)



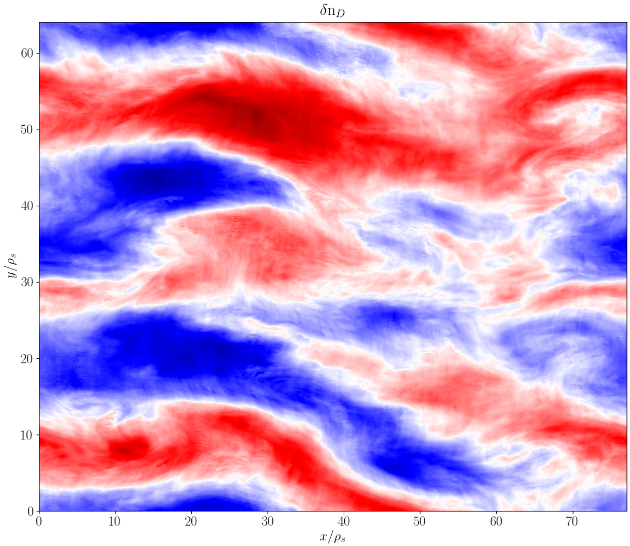
TACC
TEXAS ADVANCED COMPUTING CENTER

NERSC

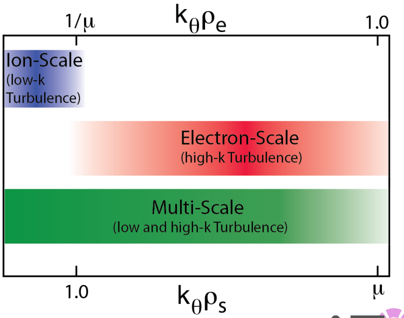
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

CGYRO Multiscale Simulation: Largest GK simulation in history

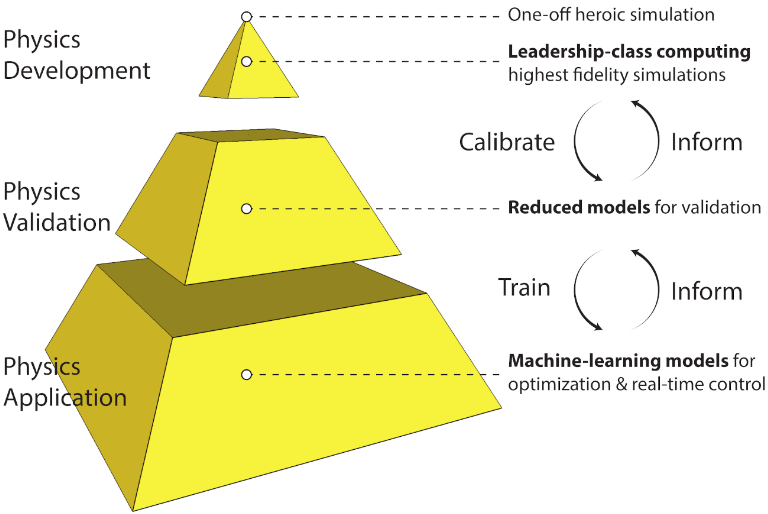


- Highest GK resolution ever
- 280M core hours on Titan
- 220K FFTs/step of length 5.6M
- 500K steps

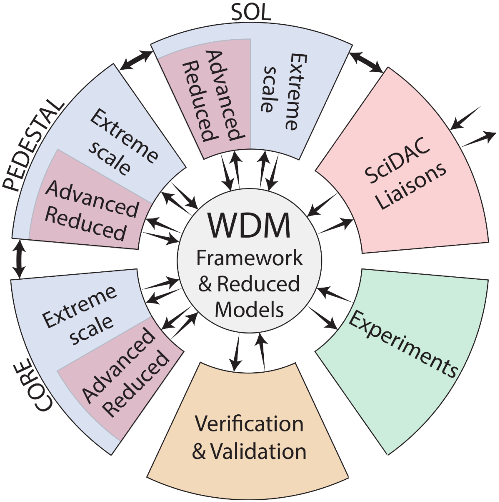


Fidelity Hierarchy is CRITICAL

Range of models from leadership codes to REDUCED MODELS



AToM SciDAC-4: Framework for integrated tokamak simulation



1. Access to experimental data
2. Outreach (liaisons) to other SciDACs
3. Verification and validation, UQ, machine learning
4. Support HPC components
5. Framework provides glue

GA supplies HPC and reduced models to international community

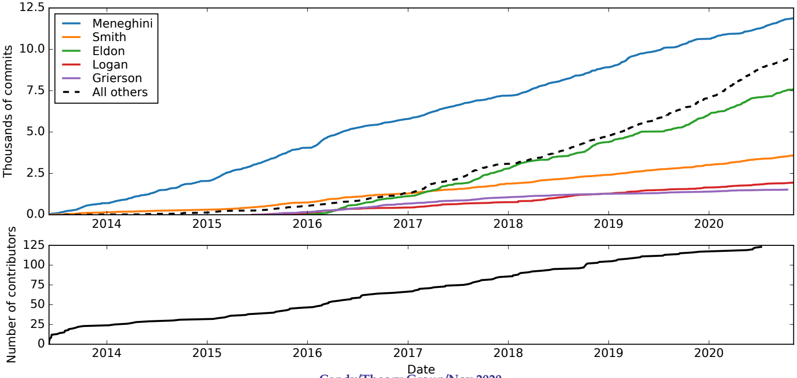
- HPC codes: CGYRO, TGYRO, NEO
- Reduced models: TGLF, EPED, EFIT
- Frameworks: OMFIT
- Users:
  - Universities: MIT, UCSD, UCLA, UW-Madison, UT-Austin, William & Mary
  - National Labs: PPPL, LLNL, ORNL
  - International: ITER (France), UKAEA, Univ. Oxford (UK), Max Planck (Germany), Chalmers (Sweden), NFRI (Korea), CEA (France)

OMFIT adoption is growing at fusion institutions worldwide

900+ total users worldwide
25k graphical sessions each year
Public installations available at 18 facilities

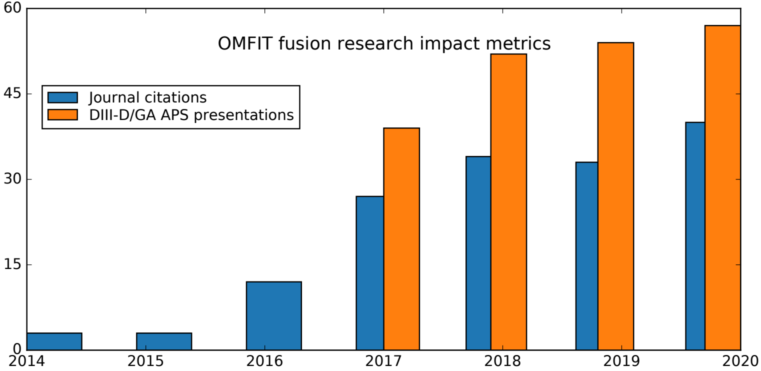
OMFIT developers base is ever expanding

- ~13% of users become developers
- Now 120 developers from 34 internatioinal institutions
- Efficient project managment achieved via decentralized development, community self-support, and heavy use of automation

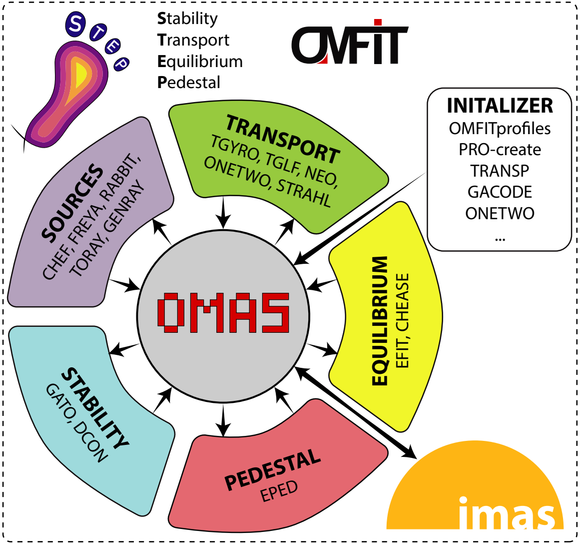


OMFIT is actively used for leading edge fusion research

- 160+ publications cite OMFIT 2013 and 2015 papers
- Each year 50+ DIII-D/GA APS presentations rely on OMFIT for their work



OMFIT has embraced the ITER IMAS data schema – what is becoming the standard "language" for fusion modeling



- OMAS library used to organize data according to IMAS schema in OMFIT
  - to achieve centralized data exchange
  - to generalized physics modules that were previously machine specific
- Use of OMAS is embodied in OMFIT STEP module for self-consistent predictions of plasma scenarios
  - open-loop, closed-loop, and optimization workflows
  - plug and play physics codes
  - machine agnostic

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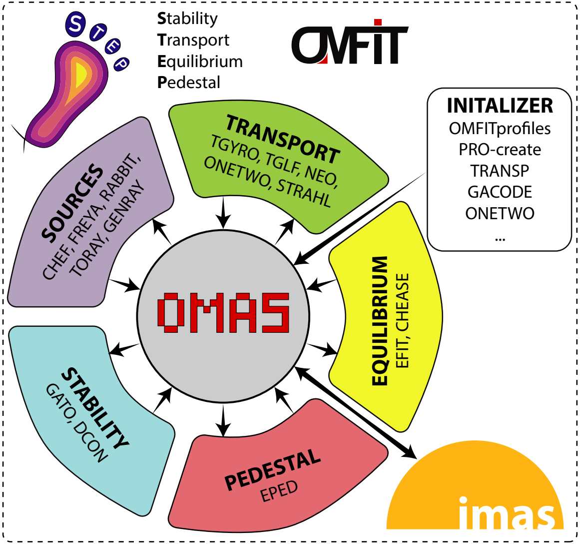
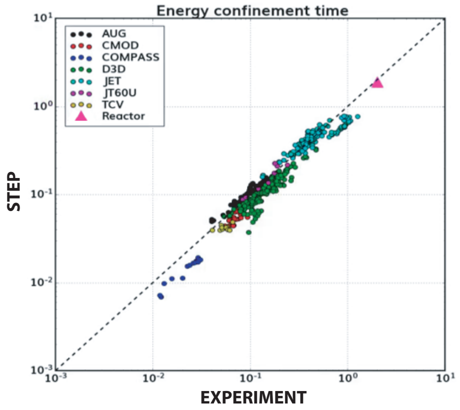


STEP was validated against multi-machine ITER98y2 database and DIII-D discharges



ALMA: New theory enables next-gen fluid compute capability

- Innovative re-thinking of plasma fluid equations allows
  - Satisfy physics properties of models to machine precision
  - Use simple and inexpensive algorithms
  - Robust simulations out-of-the-box

[Halpern and Waltz, Phys. Plasmas (2018)]: Editor's choice

[Halpern, Phys. Plasmas (2020)]: Cover, Editor's choice

[Halpern et al., JCP (2020)]: Submitted

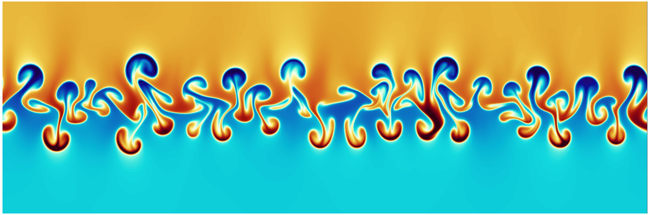


Figure: Rayleigh-Taylor instability in neutral fluid

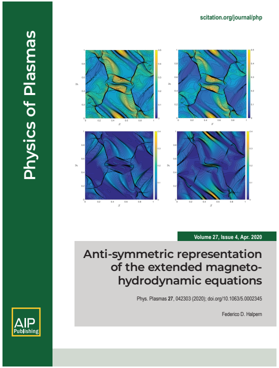
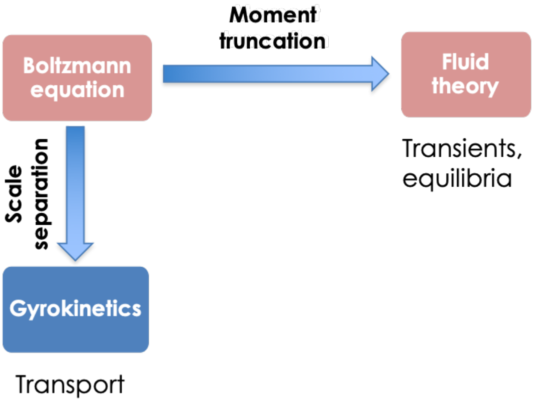


Figure: PoP cover for time-reversible MHD simulations

New ALMA code designed from ground up for exascale computers

- Started in 2017 as successor to GBS edge fluid code (Lausanne) [Halpern, JCP (2016)]
- Merge new ideas with long-standing GA effort to develop 6D kinetics
  - @Jeff place examples here… Cyclokinetics, 2015 APS invited, paper with Hirvijoki, etc



- Address DOE-FES grand-challenge of merging kinetic and MHD scales
- Evolve kinetic (transport) and MHD (equilibrium) scales under same consistent description
- Increase physics fidelity with more available compute resources

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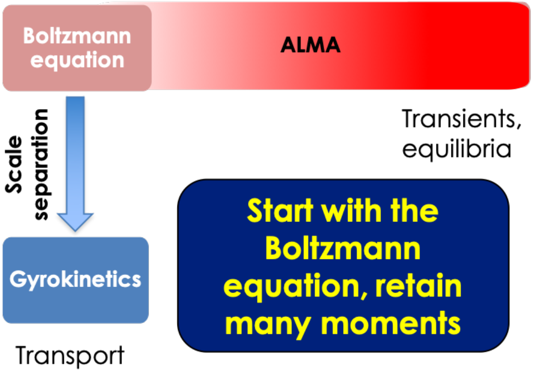

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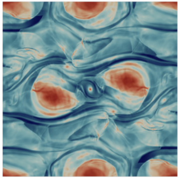
General purpose massively parallel fluid toolkit enables large scale simulations of many different physics

Solver Algorithms
- Numerical gradients
- Time integration
- Poisson solver

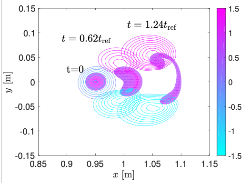
Compute infrastructure
- GPU acceleration
- Diagnostics
- Cluster communications

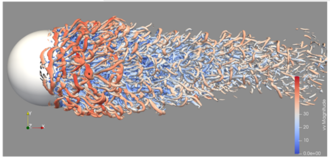
Physics problem (User)
- Model equations



MHD

Plasma turbulence



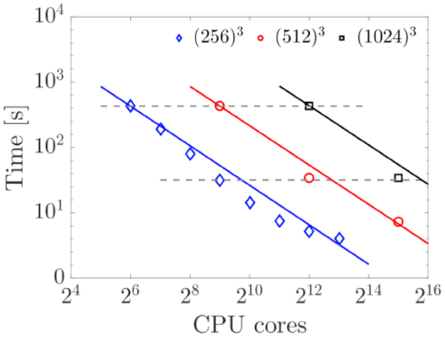


Air flow

ALMA performance on US leadership systems

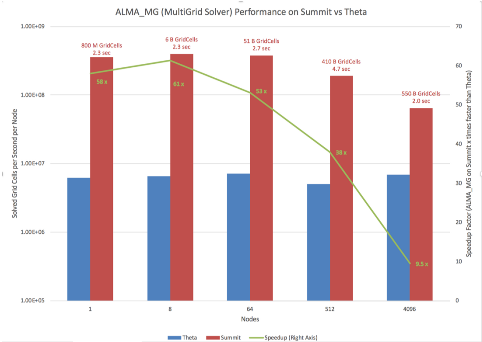
ALMA MHD code on 32k cores @ NERSC

with better than perfect scaling



ALMA Poisson solver 10-60x faster

in Summit (GPU) vs. Theta



- Fastest and most scalable fluid code in MFE community
- Crossover potential to ECP/ASCR for Poisson solver (hypre, trilinos, ...)

Ongoing applications and future ALMA plans

- Aerodynamics simulations in collaboration with GA-ASI
  - R.Stefan, 1 year development+V&V IR&D project (2021)
  - Collaborative proposal w/ASI and OSU for ONR (2021)
- Plasma shaping using curvilinear coordinates
  - F.Halpern, ongoing
- Electromagnetic tokamak turbulence simulations
  - F.Halpern, 1 year development+V&V project under IR&D (2021)
- Kinetic extensions for fluid models using GRBFs
  - F.Halpern and R.Waltz, baseline theory grant, ongoing
- Possible after *significant* investment (1+ FTE/project):
  - Simulations of EM waves in a cavity (Finite-Difference Time-Domain code)
  - Rayleigh-Taylor simulations for ICF
  - MHD simulations of Z-pinch