

**SciDAC GSEP**  
**Gyrokinetic Simulation of Energetic Particle Turbulence and Transport**  
**DE-FC02-08ER54976**

**Final Report, 12/30/2017**

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**Project webpage: <http://phoenix.ps.uci.edu/gsep/>**

## **I. Background**

Energetic particle (EP) confinement is a key physics issue for burning plasma experiment ITER, the crucial next step in the quest for clean and abundant energy, since ignition relies on self-heating by energetic fusion products ( $\alpha$ -particles). Due to the strong coupling of EP with burning thermal plasmas, plasma confinement property in the ignition regime is one of the most uncertain factors when extrapolating from existing fusion devices to the ITER tokamak. EP population in current tokamaks are mostly produced by auxiliary heating such as neutral beam injection (NBI) and radio frequency (RF) heating. Remarkable progress in developing comprehensive EP simulation codes and understanding basic EP physics has been made by two concurrent SciDAC EP projects GSEP funded by the Department of Energy (DOE) Office of Fusion Energy Science (OFES), which have successfully established gyrokinetic turbulence simulation as a necessary paradigm shift for studying the EP confinement in burning plasmas. Verification and validation have rapidly advanced through close collaborations between simulation, theory, and experiment. Furthermore, productive collaborations with computational scientists have enabled EP simulation codes to effectively utilize current petascale computers and emerging exascale computers.

## **II. Accomplishments**

We review here key physics progress in the GSEP projects regarding verification and validation of gyrokinetic simulations, nonlinear EP physics, EP coupling with thermal plasmas, and reduced EP transport models. Advances in high performance computing through collaborations with computational scientists that enable these large scale electromagnetic simulations are also highlighted. These results have been widely disseminated in numerous peer-reviewed publications including many *Phys. Rev. Lett.* papers and many invited presentations at prominent fusion conferences such as the biennial International Atomic Energy Agency (IAEA) Fusion Energy Conference and the annual meeting of the American Physics Society, Division of Plasma Physics (APS-DPP).

### **1. Verification and validation of gyrokinetic simulation of EP instabilities**

**RSAE Validation**— A verification and validation study was carried out for a sequence of reversed shear Alfvén eigenmode (RSAE) instability time slices of DIII-D discharge (#142111) in which many such frequency up-sweeping modes were observed. The mode frequency increases in time as the minimum ( $q_{\min}$ ) in the safety factor profile decreases. Calculations of the frequency and mode structure evolution from two gyrokinetic codes, GTC and GYRO, and a gyro-Landau fluid code TAEFL are compared. The three models reproduce the frequency up-sweep event within  $\pm 10\%$  of each other, and the average of the code predictions is within  $\pm 8\%$  of the measurements (**Fig. 1**); growth rates are predicted that are consistent with the observed spectral line widths.

**Fig. 1.** Variation of real frequency and growth rate among simulation models, and in DIII-D shot # 142111.

**TAE radial localization**— GTC linear simulation of DIII-D experiment finds a radial localization of toroidal Alfvén eigenmode (TAE) due to the non-perturbative EP contribution. The EP-driven TAE has a radial mode width much smaller than that predicted by MHD theory. The TAE radial position peaks at and moves with the location of the strongest EP pressure gradients (Fig. 2). Experimental data confirms that the eigenfunction drifts quickly outward in the radial direction. The non-perturbative EP contribution also breaks the radial symmetry of the ballooning mode structure and induces a dependence of the TAE frequency on toroidal mode number, in excellent agreement with experimental measurements.

**Fig. 2.** (a) Contour plot of electron temperature perturbation ( $\delta T_e$ ) on a poloidal plane from GTC simulation of TAE. (b) Comparison  $\delta T_e$  structure from simulation (left) and from DIII-D experiment (right).

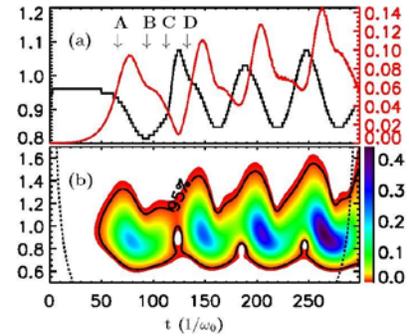
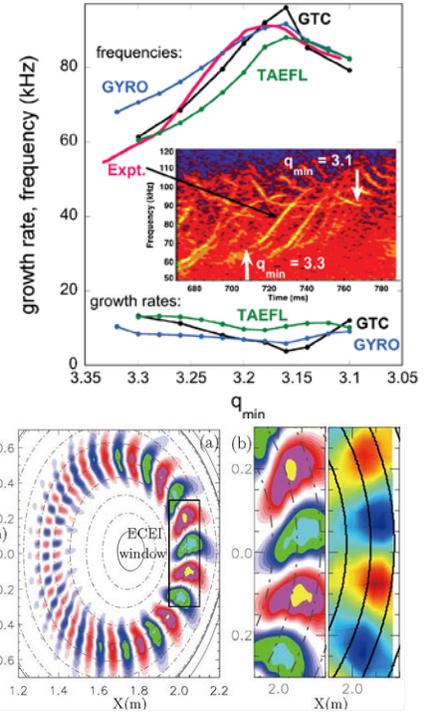
**Effects of non-axisymmetric equilibrium--** 3D effects are now ubiquitous to all toroidal magnetic confinement devices. We have adapted GTC to 3D VMEC equilibria and successfully applied to LHD, W7-X, and NSTX-RWM. Code comparisons were made with the MEGA hybrid MHD model of Y. Todo at NIFS. Both linear and, more recently, nonlinear simulations have been carried out.

## 2. Nonlinear dynamics of EP instability

**Nonlinear oscillations of BAE amplitude and frequency--** Increased EP transport by Alfvén eigenmodes has been correlated with a fast frequency oscillation (chirping) with a sub-millisecond period that has been observed in many experiments. A nonlinear oscillation of frequency and amplitude with phase shift of about  $90^\circ$  has been found by GTC simulations of beta-induced Alfvén eigenmodes (BAE) without sources and sinks in toroidal plasmas. The fast and repetitive frequency chirping (Fig. 3) is induced by the evolution of coherent structures in the EP phase space. The dynamics of the coherent structures are controlled by the competition between nonlinear particle trapping and linear free streaming. The particle and wave dynamics are intrinsically two-dimensional.

**Fig. 3.** Time evolution of (a) BAE amplitude  $|e\delta\phi/T_i|$  (red) and dominant frequency  $\omega$  (black), and (b) frequency power spectrum in GTC simulation. The y-axis on the left is  $\omega/\omega_0$ . The unit of the power intensity in panel (b) is arbitrary.

**Nonlinear interactions of BAE and BAAE**— The BAE and beta-induced Alfvén-acoustic eigenmode (BAAE) are low frequency modes that have strong interactions with both thermal and energetic particles. GTC simulation finds that BAAE can be excited by realistic EP density gradient, and that BAE and BAAE can coexist with similar linear growth rates. At the nonlinear stage, BAE modes saturate first, while BAAE modes continue to grow until nonlinear modes with a beat wave (sum of BAE and BAAE frequency) are excited. In the long time simulation, amplitudes of BAE, BAAE, and beat waves oscillate, indicating nonlinear transfers of mode energy.



### 3. Simulation code development

We have developed a multi-physics GTC code to carry out large scale EP physics simulation. Thanks to interdisciplinary and multi-institutional collaborations, GTC has incorporated in a single production version many important physical processes, i.e., microturbulence, mesoscale EP instabilities, macroscopic MHD modes, RF waves, and collisional (neoclassical) transport.

#### Current GTC physics capability needed for ISEP framework—

(1) *Three kinetic models*: Gyrokinetic (for thermal and fast ions) or drift kinetic (for thermal or fast electrons), fully-kinetic particles, and fluid-kinetic hybrid electron model (for thermal electrons). Particle species can use either full- $f$  simulation or  $\delta f$  formulation with linearized Fokker-Planck collision operators conserving particle, momentum, and energy.

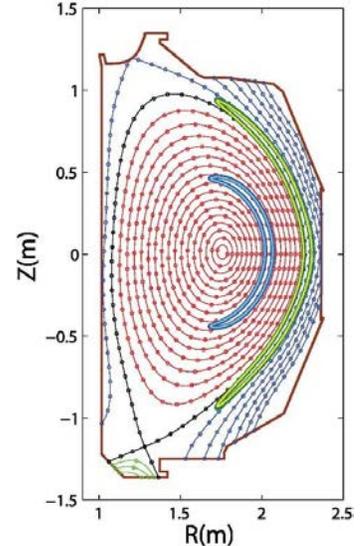
(2) *Three fluid models*: Reduced resistive MHD, massless and finite-mass electron fluid model.

(3) *Global toroidal geometry*: GTC interfaces with MHD equilibrium solvers EFIT, VMEC, and M3D-C1 for both tokamaks and stellarators. In core simulations, a field-aligned mesh using magnetic coordinates in the real space provides maximal numerical efficiency without any geometry approximation. A recent upgrade enables global simulations coupling the core and SOL across the separatrix by using cylindrical coordinates with field-aligned particle-grid interpolation. GTC interfaces with TRANSP and ONETWO for experimental profiles with equilibrium current, radial electric field, plasma rotations, and sources.

**Fig. 4.** GTC computational grids on a poloidal plane coupling core and SOL, and fully kinetic and guiding center calculations of two EP orbits in DIII-D shot #158103.

(4) *Three field solvers*: the gyrokinetic Poisson equation for the electrostatic potential is discretized in real space using the finite difference or finite element method for either the integral form or the Pade approximation. The resulting sparse matrix is solved by either PETSc or *hypra* package. The parallel magnetic perturbation is solved using perpendicular force balance, and the Ampere's law is solved for the parallel vector potential.

(5) *Synthetic diagnostics*: GTC interfaces with the Synthetic Diagnostics Platform (SDP), which currently has reflectometry, electron cyclotron emission, and beam emission spectroscopy.



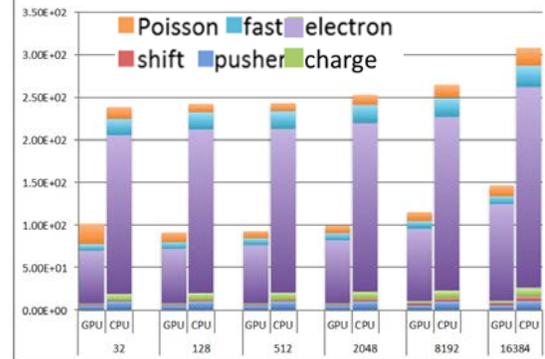
#### Current GTC computational capability--

Thanks to closed collaborations with computational scientists, GTC carried out the first fusion production simulations at tera-scale in 2001 and at peta-scale in 2008, and to fully utilize the heterogeneous architectures using *NVIDIA* GPU (graphic processing unit) accelerators in 2011, and using *Intel* MIC (many integrated core) co-processors on in 2013. GTC is one of the two fusion codes selected by the Center for Accelerated Application Readiness (CAAR), a DOE Office of Advanced Scientific Computing Research (ASCR) program to prepare prominent codes across all DOE supported research portfolio for the emerging exascale computers such as the next generation computer Summit at ORNL.

*Multiple levels of parallelism*: GTC uses MPI domain decomposition, particle decomposition, and OpenMP shared memory partitioning to scale up to millions of cores and take advantage of the memory hierarchy of current generation parallel computers.

*GPU optimization:* The computationally expensive particle subroutines are fully ported and optimized on GPU for all particle species using OpenACC. GTC shows near-ideal weak scaling performance up to the full Titan (the fastest computer in US) at ORNL using physics simulation parameters. GTC has achieved an unprecedented speed of pushing  $1.5 \times 10^{11}$  particles with  $2.5 \times 10^6$  grids for 1 time step in less than 1 second wall-clock time using 16,384 GPUs (88% of Titan) as shown in **Fig. 5**, thanks to optimization by ASCR CAAR collaborations. GTC was recently ported to Summitdev, the prototype computer of Summit at ORNL, and demonstrated the expected GPU speed increase as discussed in Sec. 5.

**Fig. 5:** GTC weak scaling on Titan from simulations using DIII-D parameters. X-axis is node number. Y-axis is wall-clock time (second) after 150 time steps.



*MIC optimization:* GTC using OpenMP 4.0 for Intel many integrated cores (MIC) has an excellent weak scalability [WangE16]. More optimizations are discussed in Sec. 5 on Computational Partnership.

### III. Publications

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4. [Full Torus Electromagnetic Gyrokinetic Particle Simulations with Kinetic Electrons](#), Y. Nishimura, Z. Lin and L. Chen, *Commun. Comput. Phys.* **5**, 183 (2009).
5. [Turbulent transport of trapped electron modes in collisionless plasmas](#), Yong Xiao and Zhihong Lin, *Phys. Rev. Lett.* **103**, 085004 (2009).
6. [Properties of microturbulence in toroidal plasmas with reversed magnetic shear](#), Wenjun Deng and Zhihong Lin, *Phys. Plasmas* **16**, 102503 (2009).
7. [The importance of parallel nonlinearity in the self-interaction of geodesic acoustic mode](#), H. S. Zhang, Z. Qiu, L. Chen, and Z. Lin, *Nuclear Fusion* **49**, 125009 (2009).
8. [Electromagnetic formulation of global gyrokinetic particle simulation in toroidal geometry](#), I. Holod, W. L. Zhang, Y. Xiao, and Z. Lin, *Phys. Plasmas* **16**, 122307 (2009).
9. [Effects of electron dynamics in toroidal momentum transport driven by ion temperature gradient turbulence](#), I. Holod and Z. Lin, *Plasma Phys. Contr. Fusion* **52**, 035002 (2010).
10. [Fluctuation characteristics and transport properties of collisionless trapped electron mode turbulence](#), Yong Xiao, Ihor Holod, Wenlu Zhang, Scott Klasky, and Zhihong Lin, *Phys. Plasmas* **17**, 022302 (2010).
11. [Scalings of energetic particle transport by ion temperature gradient Microturbulence](#), Wenlu Zhang, Viktor Decyk, Ihor Holod, Yong Xiao, Zhihong Lin, and Liu Chen, *Phys. Plasmas* **17**, 055902 (2010).
12. [Trapped Electron Damping of Geodesic Acoustic Mode](#), Huasen Zhang and Zhihong Lin, *Phys. Plasmas* **17**, 072502 (2010).
13. [Gyrokinetic Simulation of Turbulence Driven Geodesic Acoustic Modes in Edge Plasmas of HL-2A Tokamak](#), Feng Liu, Z. Lin, J. Q. Dong, K. J. Zhao, *Phys. Plasmas* **17**, 112318 (2010).
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16. [Gyrokinetic simulation of magnetic compressional modes in general geometry](#), Peter Porazik and Zhihong Lin, *Commun. Comput. Phys.* **10**, 899 (2011).
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19. [Comment on "Electrostatic and magnetic transport of energetic ions in turbulent plasmas"](#), W. L. Zhang, Z. Lin, and L. Chen, *Phys. Rev. Lett.* **107**, 239501 (2011).
20. [Gyrokinetic simulation model for kinetic magnetohydrodynamic processes in magnetized plasmas](#), W. Deng, Z. Lin, and I. Holod, *Nuclear Fusion* **52**, 023005 (2012).
21. [Turbulent Transport of Toroidal Angular Momentum in Fusion Plasmas](#), I. Holod, Z. Lin, and Y. Xiao, *Phys. Plasmas* **19**, 012314 (2012).
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25. [Verification and validation of linear gyrokinetic simulation of Alfvén eigenmodes in the DIII-D tokamak](#), D. A. Spong, E. M. Bass, W. Deng, W. W. Heidbrink, Z. Lin, B. Tobias, M. A. Van Zeeland, M. E. Austin, C. W. Domier, N. C. Luhmann, Jr., *Phys. Plasmas* **19**, 082511 (2012).
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28. [Verification of Electromagnetic Fluid-Kinetic Hybrid Electron Model in Global Gyrokinetic Particle Simulation](#), I. Holod and Z. Lin, *Phys. Plasmas* **20**, 032309 (2013).
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31. [Radial Localization of Toroidicity-Induced Alfvén Eigenmodes](#), Zhixuan Wang, Zhihong Lin, Ihor Holod, W. W. Heidbrink, Benjamin Tobias, Michael Van Zeeland, and M. E. Austin, *Phys. Rev. Lett.* **111**, 145003 (2013).
32. [Does the orbit-averaged theory require a scale separation between periodic orbit size and perturbation correlation length?](#) Wenlu Zhang and Zhihong Lin, *Phys. Plasmas* **20**, 102306 (2013).
33. [Verification of particle simulation of radio frequency waves in fusion plasmas](#), A. Kuley, Z. X. Wang, Z. Lin, and F. Wessel, *Phys. Plasmas* **20**, 102515 (2013).
34. [Nonlinear generation of zonal fields by the beta-induced Alfvén eigenmode in tokamak](#), H. S. Zhang and Z. Lin, *Plasma Sci. Technol.* **15**, 969 (2013).
35. [Microturbulence in DIII-D Tokamak Pedestal. I. Electrostatic Instabilities](#), D. Fulton, Z. Lin, I. Holod, and Y. Xiao, *Phys. Plasmas* **21**, 042110 (2014).
36. [Particle simulation of lower hybrid wave propagation in fusion plasmas](#), J. Bao, Z. Lin, A. Kuley, and Z. X. Lu, *Plasma Phys. Contr. Fusion* **56**, 095020 (2014).

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38. [Effects of magnetic islands on drift wave instability](#), P. Jiang, Z. Lin, I. Holod, and C. Xiao, *Phys. Plasmas* **21**, 122513 (2014).
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44. [Method to integrate full particle orbit in toroidal plasmas](#), X. S. Wei, Y. Xiao, A. Kuley, and Z. Lin, *Phys. Plasmas* **22**, 092502 (2015).
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50. [Gyrokinetic particle simulation of fast-electron driven beta-induced Alfvén eigenmode](#), Junyi Cheng, Wenlu Zhang, Zhihong Lin, Ihor Holod, Ding Li, Yang Chen, and Jintao Cao, *Phys. Plasmas* **23**, 052504 (2016).
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63. [Excitation of Low Frequency Alfvén Eigenmodes in Toroidal Plasmas](#), Yaqi Liu, Zhihong Lin, Huasen Zhang, Wenlu Zhang, *Nuclear Fusion* **57**, 114001 (2017).
64. [Gyrokinetic particle simulations of the effects of compressional magnetic perturbations on drift-Alfvénic instabilities in tokamaks](#), Ge Dong, Jian Bao, Amitava Bhattacharjee, Alain Brizard, Zhihong Lin, and Peter Porazik, *Phys. Plasmas* **24**, 081205 (2017).
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66. [Drift-wave Stabilities in the Field-Reversed Configuration](#), C. K. Lau, D. P. Fulton, I. Holod, Z. Lin, M. Binderbauer, T. Tajima, and L. Schmitz, *Phys. Plasmas* **24**, 082512 (2017).
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68. [A conservative scheme of drift kinetic electrons for gyrokinetic simulation of kinetic-MHD processes in toroidal plasmas](#), J. Bao, D. Liu, Z. Lin, *Phys. Plasmas* **24**, 102516 (2017).

#### IV. Invited Presentations at Professional Conferences

- 2008 -- SciDAC Gyrokinetic Particle Simulation Workshop, Irvine, USA;  
 -- Cray Technical Workshop, San Francisco, USA;  
 -- 21<sup>st</sup> US Transport Task Force Workshop, Boulder, USA;  
 -- International West Lake Workshop on Fusion Theory and Simulation, Hangzhou, China.
- 2009 -- 4<sup>th</sup> IAEA Technical Meeting (IAEA-TM) on the Theory of Plasma Instabilities, Kyoto, Japan;  
 -- Scientific Discovery through Advanced Computing Program (SciDAC) 2009 Conference, San Diego, USA;  
 -- Plenary talk, Joint US-European Transport Task Force Workshop, San Diego, USA;  
 -- 36<sup>th</sup> EPS Conference on Plasma Physics, Sofia, Bulgaria (delivered by Ihor Holod);  
 -- 21<sup>st</sup> International Conference on Numerical Simulation of Plasmas, Lisbon, Portugal (delivered by Wei-li Lee);  
 -- International Sherwood Fusion Theory Conference, Denver, USA (Invited talk by Xiao Yong);  
 -- 51<sup>st</sup> Annual Meeting of the APS Division of Plasma Physics, Atlanta, USA (Invited talk by Wenlu Zhang);  
 -- SciDAC Workshop on Plasma Turbulence and Energetic Particles, Irvine, USA.
- 2010 -- 7<sup>th</sup> International Conference on Computational Physics, Beijing, China;  
 -- 23<sup>rd</sup> US Transport Task Force Workshop, Annapolis, USA (delivered by Ihor Holod);  
 -- 3<sup>rd</sup> annual SciDAC GSEP energetic particle workshop, San Diego, USA;

- International Workshop on Plasma Science and Applications, Xiamen, China;
  - 4<sup>th</sup> International Workshop on Fusion Theory and Simulation, Beijing, China;
  - International Sherwood Fusion Theory Conference, Seattle, USA (Invited talks by Wenjun Deng & Wenlu Zhang).
- 2011— Workshop on Fusion Simulation Program, San Diego, USA;
- 5<sup>th</sup> ITER International Summer School, Aix en Provence, France;
  - Chinese Summer School on Plasma Physics, CSSPP11, Dalian, China;
  - 7<sup>th</sup> joint meeting of Chinese physicists worldwide, Kaohsiung, Taiwan;
  - 12<sup>th</sup> IAEA Technical Meeting on Energetic Particles in Magnetic Confinement Systems, Austin, USA;
  - 5<sup>th</sup> IAEA Technical Meeting on Theory of Plasma Instabilities, Austin, USA (Oral presentations by Ihor Holod & Xiao Yong)
  - 22<sup>nd</sup> International Conference on Numerical Simulation of Plasmas, Long Branch, USA (Invited talk by Ihor Holod);
  - US Transport Task Force Workshop, San Diego, USA (Oral presentations by Huasen Zhang, Wenjun Deng, Peter Porazik, Yong Xiao, & Ihor Holod).
- 2012 -- US-Japan Workshop on Integrated Modeling, San Diego, USA;
- Workshop on Energetic Particle Physics, Irvine, USA;
  - US Transport Task Force Workshop, Annapolis, USA;
  - 2<sup>nd</sup> Asia Pacific Transport Working Group Annual meeting, Chengdu, China;
  - Workshop on MHD and Energetic Particles in Laboratory, Space and Astrophysical Plasmas, Kavli Institute for Astronomy and Astrophysics, Peking University, China;
  - Magnetic Fusion Theory and Simulation Workshop, Hefei, China;
  - 9<sup>th</sup> Meeting of the ITPA Energetic Particle Topical Group, San Diego, USA;
  - International Sherwood Fusion Theory Conference, Atlanta, USA (Invited talk by Huasen Zhang);
  - Joint Varenna - Lausanne International Workshop on Theory of Fusion Plasmas, Varenna, Italy (Invited talk by Ihor Holod, Yong Xiao).
- 2013 -- 12<sup>th</sup> Asia Pacific Physics Conference (APPC12), Chiba, Japan;
- 23<sup>rd</sup> International TOKI Conference (ITC-23) on Large-scale Simulation on Fusion Science, Toki, Japan;
  - Summary talk, 13<sup>th</sup> IAEA Technical Meeting on Energetic Particles in Magnetic Confinement Systems, Beijing, China;
  - DOE Technical Program Review: Large Scale Production Computing and Storage Requirements for Fusion Energy Sciences, Rockville, USA;
  - U.S. - E.U. Joint Transport Task Force Workshop, Santa Rosa, USA;
  - Fusion Simulation Workshop, Beijing, China;
  - 23<sup>rd</sup> International Conference on Numerical Simulation of Plasmas (23<sup>rd</sup> ICNSP), Beijing, China (Invited talk by Ihor Holod);
  - International Sherwood Fusion Theory Conference, Santa Fe, USA (Invited talk by Zhixuan Wang).
- 2014 -- 2<sup>nd</sup> annual Workshop on Fusion Simulation, Chengdu, China;
- Plenary talk, Transport Task Force Workshop, San Antonio, USA;
  - 11<sup>th</sup> Asia Pacific Plasma Theory Conference (APPTC), Jeju, Korea;
  - 4<sup>th</sup> East-Asian School and Workshop on Laboratory, Space, Astrophysical Plasmas, Harbin, China;
  - 25<sup>th</sup> International Conference on Plasma Physics and Controlled Nuclear Fusion Research, International Atomic Energy Agency, Saint Petersburg, Russia;
  - 56<sup>th</sup> Annual Meeting of American Physical Society, Division of Plasma Physics, New Orleans, USA (Invited talk by Zhixuan Wang);
- 2015 -- Plenary talk, Transport Task Force Workshop, Salem, USA;

- 3<sup>rd</sup> Annual Workshop on Fusion Simulation, Hefei, China;
- 57<sup>th</sup> Annual Meeting of American Physical Society, Division of Plasma Physics, Savannah, USA  
(Invited talk by Daniel Fulton);
- 7<sup>th</sup> IAEA Technical Meeting on Theory of Plasma Instabilities, Frascati, Italy (Oral presentations  
by Ihor Holod)
- 24<sup>th</sup> International Conference on Numerical Simulation of Plasmas (24<sup>th</sup> ICNSP), Colorado, USA  
(Invited talk by Jian Bao);
- 2016 -- Transport Task Force Workshop, Denver, USA;
- DOE Exascale Requirements Review for Fusion Energy Sciences, DC, USA;
- 4<sup>th</sup> Annual Workshop on Fusion Simulation, Hangzhou, China;
- 12<sup>th</sup> Asia Pacific Plasma Theory Conference, Hangzhou, China.
- 2017 -- Transport Task Force Workshop, Williamsburg, USA (plenary talk by Yaqi Liu);
- DOE Exascale Requirements Review for Fusion Energy Sciences, DC, USA;
- 5<sup>th</sup> Annual Workshop on Fusion Simulation, Beijing, China;
- 8<sup>th</sup> IAEA Technical Meeting on Theory of Plasma Instabilities, Vienna, Austria;
- 15<sup>th</sup> IAEA Technical Meeting on Energetic Particles in Magnetic Confinement Systems,  
Princeton, USA.