DISCLAIMER

SciDAC ISEP: Integrated Simulation of Energetic Particles in Burning Plasmas

DE-SC0018270, 9/1/2017-8/31/2023

Final report

1. Abstract summarizing the general topics addressed during the award.

The objective of the SciDAC Center for Integrated Simulation of Energetic Particles in Burning Plasmas (ISEP) is to improve physics understanding of energetic particle (EP) confinement and EP interactions with burning thermal plasmas through large-scale simulations. The ISEP center will develop a multiscale and multiphysics ISEP framework for a predictive capability of EP physics and deliver an EP module incorporating both first-principles simulations and high fidelity reduced transport models to the fusion whole device modeling (WDM) project.

The ISEP framework will enable us to perform long time, global kinetic simulations of EP physics in burning plasmas, by utilizing the full power of the next generation supercomputers. Our research and development activities will build on fruitful collaborations with computer scientists and applied mathematicians to offer enabling technologies for performance scalability, portability, solvers, coupling for integration with the fusion WDM project, and long-term preservation of data.

2. Brief technical description of most relevant projects/publications.

Significant progress has been made by the SciDAC-4 ISEP (Integrated Simulation of Energetic Particle) project, which has developed large scale simulations using global gyrokinetic and kinetic-MHD codes with rigorous verification and validation to improve our understanding of EP transport driven by EP instabilities and EP coupling with microturbulence. These first-principles simulations have facilitated development of high-fidelity reduced EP transport models and deep learning models. The progress has been enabled by fruitful collaborations with computer scientists and applied mathematicians on enabling technologies for performance scalability, portability, solvers, and coupling for integration with fusion whole device modeling. These simulations have effectively utilized Department of Energy (DOE) leadership computing facility including INCITE, ALCC, and NERSC awards to the ISEP project. The ISEP Center leads the EP research in the world fusion energy program, specifically,

- Paradigm shift to integrated gyrokinetic simulations of EP turbulence
- First reduced models for EP transport
- Largest collaboration on predicting alpha-particle confinement in ITER scenarios

Global gyrokinetic code GTC has been continuously developed as a comprehensive platform for integrated simulation of turbulence and transport in burning plasmas. Based on gyrokinetic formulation, GTC has incorporated in a single production version many important physical processes in fusion plasmas, i.e., microturbulence, energetic particle (EP) instabilities such as Alfven eigenmodes (AE)/fishbones, MHD modes such as kink and tearing modes, and collisional (neoclassical) transport, with extensive validation by existing experiments. GTC is the only global gyrokinetic code in the world fusion program that has demonstrated full electromagnetic nonlinear simulations including shear and compressible magnetic perturbations and equilibrium current, which are important for cross-scale interactions. GTC has been extensively verified and validated for simulations of neoclassical and turbulent transport, AE/fishbones, and ideal/resistive MHD modes in tokamaks including DIII-D, JET, ADITYA-U, EAST, KSTAR, HL-2A and ITER, spherical tokamaks including NSTX-U, MAST-U and ST40, stellarators including W7-X and LHD, and FRC experiments C-2U. GTC interfaces with MHD equilibrium solvers EFIT, VMEC, and M3D-C1 for realistic magnetic geometry, and with the Synthetic Diagnostics Platform (SDP) for reflectometry, electron cyclotron emission, and beam emission spectroscopy. A field-aligned mesh using magnetic coordinates in real space provides maximal numerical efficiency without geometry approximation. We have also implemented energetic particle distribution function using anisotropic slowing-down distribution and numerical distribution using constants of motion, and a full-f simulation model using constants of motion for long time simulation.

GTC cross-scale simulations using kinetic electrons with real electron-to-ion mass ratio have been enabled by effectively using the world's fastest supercomputers, thanks to continued multidisciplinary collaborations with computational partnerships supported by DOE SciDAC and INCITE/ALCC over the past two decades. Recently, GTC has been optimized for NVIDIA GPU on Perlmutter computer at NERSC in collaboration with NVIDIA, for AMD GPU on the exascale computer Frontier at ORNL in collaboration with AMD, and for Intel GPU on the exascale computer Aurora at ANL in collaboration with Intel. The followings are some examples of validation of GTC cross-scale simulations of AE in tokamak.

- *Regulation of Alfven eigenmodes by microturbulence in fusion plasmas*, P. Liu, X. Wei, Z. Lin, G. Brochard, G.J. Choi, W.W. Heidbrink, J.H. Nicolau, and G. R. McKee, *Phys. Rev. Lett.* **128**, 185001 (2022).

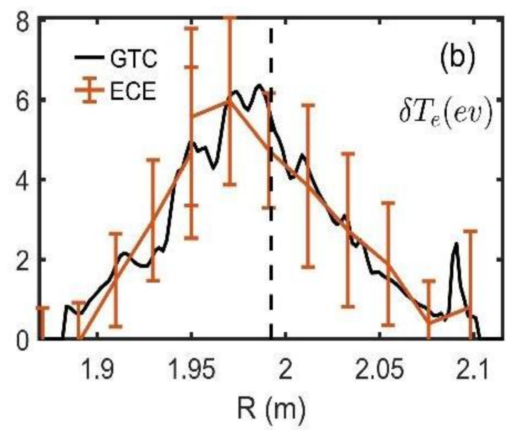

Fig. 1. *Radial profiles of temperature perturbation δT_e from GTC simulations and ECE measurements of RSAE in DIII-D shot #159243.*

GTC electromagnetic simulations using kinetic electrons with real electron-to-ion mass ratio find that microturbulence can play a critical role in regulating reversed shear Alfven eigenmode (RSAE), even though the microturbulence directly drives little EP transport due to gyro-averaging effects as expected by the conventional wisdom. The AE amplitude in the quasisteady state from simulations coupling AE and microturbulence, for the first time, agrees very well with experimental measurements (**Fig. 1**).

- *Saturation of fishbone instability by self-generated zonal flows in tokamak plasmas*, G. Brochard, C. Liu, X. Wei, W. Heidbrink, Z. Lin, N. Gorelenkov, J. Bao, A. R. Polevoi, M. Schneider, S. H. Kim, S. D. Pinches, P. Liu, J. H. Nicolau, and H. Lutjens, *Phys. Rev. Lett.* **132**, 075101 (2024).

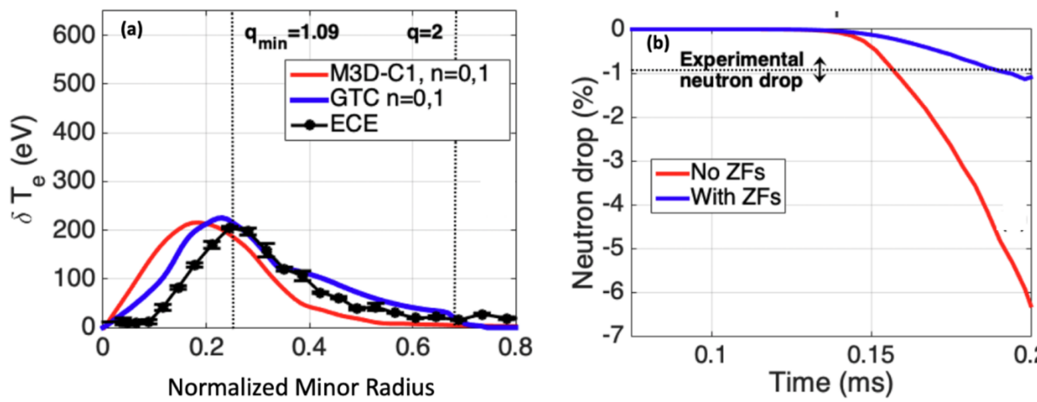

Fig. 2. *(a) Comparison of measured radial eigenfunction measured by ECE in DIII-D shot #178631 (black) with the fishbone eigenfunction calculated by GTC (blue) and by M3D-C1 (red) when zonal flows are included. (Without zonal flows the agreement is poor.) (b) Drop in neutron rate at the fishbone burst as calculated by GTC with (blue) and without (red) zonal flows included. The calculation with zonal flows is consistent with the measured drop.*

Fig. 2 shows a GTC simulation of a DIII-D discharge in which the fishbone became unstable. The safety factor q-profile was accurately known and resembles the profiles predicted for the ITER baseline; other plasma profiles were also accurately measured. After processing by a synthetic diagnostic, the simulated radial eigenfunction compares well with the radial eigenfunction measured by an electron cyclotron emission diagnostic (Fig. 3a). Fast-ion transport is assessed by comparison with the measured drop in neutron emission at the fishbone and the simulation that includes zonal flows is in excellent agreement with experiment (Fig. 3b). In addition, the prediction that the fishbone creates a zonal flow is validated by the onset of an internal transport barrier in the ion temperature profile (not shown).

3. Paragraph indicating the number of presentations made and venues. Indicate presentations given at national labs, industry, universities, national and international professional meetings.

Invited Presentations at Professional Conferences:

2018 -- A Scientific Journey from Wakefields to Astrophysics and Fusion: A Symposium in Honor of Toshiki Tajima, Irvine, USA;
-- Transport Task Force Workshop, San Diego, USA;
-- DOE SciDAC-4 Principal Investigator Meeting, Washington DC, USA;
-- US-Japan JIFT Exascale Computing Workshop, Princeton, USA.
2019 -- DOE SciDAC-4 Principal Investigator Meeting, Washington DC, USA;
-- 10th International Conference on Computational Methods (ICCM2019), Singapore

(delivered by Klasky);
-- 16th IAEA Technical Meeting on Energetic Particles in Magnetic Confinement Systems, Shizuoka City, Japan (selected as invited talk; unable to attend);
-- 61st Annual Meeting of APS Division of Plasma Physics, Mini-Conference on Building Bridge to Exascale Computing: Applications and Opportunities for Plasma Science, Fort Lauderdale, USA;
-- US-Japan Compact Torus Workshop (CT2019), Toki, Japan;
-- Annual Meeting of Asia-Pacific Physical Society (AAPPS-DPP2019), Hefei, China;

2020 -- Annual Meeting of Asia-Pacific Physical Society (AAPPS-DPP2020) (online);

2021 -- 10th US-PRC Magnetic Fusion Collaboration Workshop (online);
-- Transport Task Force Workshop (online) (plenary talks by Pengfei Liu and Javier Nicolau);
-- International Tokamak Physics Activities (ITPA) (online);
-- 47th EPS Conference on Plasma Physics (online);
-- Platform for Advanced Scientific Computing (PASC21) Conference (online).

2022 -- US-Japan JIFT Exascale Computing Workshop (online);
-- 48th EPS Conference on Plasma Physics (online, invited talk by Guillaume Brochard);
-- Technology of Fusion Energy (TOFE2022), Anaheim, CA;
-- 27th International Tokamak Physics Activities (ITPA-EP) (online);
-- Festival de Théorie 2022, Aix-en-Provence, France;
-- 33rd IUPAP Conference on Computational Physics (online);
-- H-Mode Workshop (HMWS22) (online).

2023 -- 28th International Tokamak Physics Activities (ITPA) (online);
-- 49th European Conference on Plasma Physics, Bordeaux, France;
-- 29th International Conference on Plasma Physics and Controlled Nuclear Fusion Research, International Atomic Energy Agency, London, UK;
-- US-Japan JIFT Exascale Computing Workshop, NIFS, Japan;
-- Annual Meeting of Asia-Pacific Physical Society (AAPPS-DPP2023), Nagoya, Japan.

2024 – US-EU Transport Task Force Workshop, Asheville (invited talk by Xishuo Wei);
-- 31st International Tokamak Physics Activities (ITPA-EP) (invited talk by Yangyang Yu);
-- Fusion Energy R&D on Advanced and Long Pulse Tokamaks Principal Investigator Meeting, Norfolk;
-- 24th International Stellarator and Heliotron Workshop (ISHW24), Hiroshima, Japan.

Invited Presentations at Educational, Governmental Institutions

2018 – Princeton Plasma Physics Laboratory, USA;
-- Indian Institute of Science, Bengaluru, India;
-- MIT, USA.

2019 -- Culham Center for Fusion Energy (CCFE), UK.

2020 – Zhejiang University, Hangzhou, China (online).

2021 – Seoul National University, South Korea (online);
-- Princeton Plasma Physics Laboratory (online);
-- SoCal Plasma Zoom Seminar (UCI, UCLA, UCSD) (online);
-- Culham Center for Fusion Energy (CCFE), UK.

2022 – ITER International Organization;
-- Princeton Plasma Physics Laboratory.

2023 – National Center for High-Performance Computing, Taiwan;

2024 -- Seoul National University, South Korea.

4. Personnel Involvement.

Postdoc at UC Irvine: Guillaume Brochard, Gyung Jin Choi, Javier Nicolau, Xishuo Wei, Pengfei Liu, Jian Bao.

PhD students at UC Irvine: Wenhao Wang, Sam Taimourzadeh, Calvin Lau.

5. Unexpended funds.

None.

6. Listing of all published articles acknowledging support by the award.

1. *Simulation of toroidicity-induced Alfven eigenmode excited by energetic ions in HL-2A tokamak plasmas*, Hongda He, Junyi Cheng, J. Q. Dong, Wenlu Zhang, Chenxi Zhang, Jinxia Zhu, Ruirui Ma, T. Xie, G. Z. Hao, A. P. Sun, G. Y. Zheng, W. Chen and Z. Lin, *Nuclear Fusion* **58**, 126023 (2018).
2. *Heterogeneous Programming and Optimization of Gyrokinetic Toroidal Code Using Directives*, Wenlu Zhang, Wayne Joubert, Peng Wang, Matthew Niemerg, Bei Wang, William Tang, Sam Taimourzadeh, Lei Shi, Jian Bao, Zhihong Lin, *Lecture Notes in Computer Science* **11381**, 3–21 (2019). (WACCPD 2018 Workshop, Dallas).
3. *Gyrokinetic simulations of Toroidal Alfven Eigenmodes excited by energetic ions and external antennas on the Joint European Torus*, V. Aslanyan, S. Taimourzadeh, L. Shi, Z. Lin, G. Dong, P. Puglia, M. Porkolab, R. Dumont, S. E. Sharapov, J. Mailloux, M. Tsalas, M. Maslov, A. Whitehead, R. Scannell, S. Gerasimov, S. Dorling, S. Dowson, H. K. Sheikh, T. Blackman, G. Jones, A. Goodyear, K. K. Kirov, P. Blanchard, A. Fasoli, D. Testa, and JET Contributors, *Nuclear Fusion* **59**, 026008 (2019).
4. *Nonlinear Saturation of Kinetic Ballooning Modes by Zonal Fields in Toroidal Plasmas*, G. Dong, J. Bao, A. Bhattacharjee, and Z. Lin, *Phys. Plasmas* **26**, 010701 (2019).
5. *Effects of RMP-Induced Changes of Radial Electric Fields on Microturbulence in DIII-D Pedestal Top*, S. Taimourzadeh, L. Shi, Z. Lin, R. Nazikian, I. Holod, D. Spong, *Nuclear Fusion* **59**, 046005 (2019).
6. *Global simulation of ion temperature gradient instabilities in a field-reversed configuration*, J. Bao, C. K. Lau, Z. Lin, H. Y. Wang, D. P. Fulton, S. Dettrick, and T. Tajima, *Phys. Plasmas* **26**, 042506 (2019).
7. *Verification and validation of integrated simulation of energetic particles in fusion plasmas*, S. Taimourzadeh, E. M. Bass, Y. Chen, C. Collins, N. N. Gorelenkov, A. Konies, Z. X. Lu, D. A. Spong, Y. Todo, M. E. Austin, J. Bao, A. Biancalani, M. Borchardt, A. Bottino, W. W. Heidbrink, Z. Lin, R. Kleiber, A. Mishchenko, L. Shi, J. Varela, R. E. Waltz, G. Yu, W. L. Zhang, and Y. Zhu, *Nuclear Fusion* **59**, 066006 (2019).
8. *Global gyrokinetic simulation of microturbulence with kinetic electrons in the presence of magnetic island in tokamak*, K. S. Fang and Z. Lin, *Phys. Plasmas* **26**, 052510 (2019).
9. *Kinetic particle simulations in a global toroidal geometry*, S. De, T. Singh, A. Kuley, J. Bao, Z. Lin, G. Y. Sun, S. Sharma, and A. Sen, *Phys. Plasmas* **26**, 082507 (2019).
10. *Gyrokinetic simulations of nonlinear interactions between magnetic islands and microturbulence*, Kaisheng Fang, Jian Bao, and Zhihong Lin, *Plasma Sci. Technol.* **21**, 115102 (2019).

11. *Gyrokinetic particle simulations of interactions between energetic particles and magnetic islands induced by neoclassical tearing modes*, X. Tang, Z. Lin, W. W. Heidbrink, J. Bao, C. Xiao, Z. Li and J. Li, *Phys. Plasmas* **27**, 032508 (2020).
12. *Global Gyrokinetic Particle Simulations of Microturbulence in W7-X and LHD Stellarators*, H. Y. Wang, I. Holod, Z. Lin, J. Bao, J. Y. Fu, P. F. Liu, J. H. Nicolau, D. Spong, Y. Xiao, *Phys. Plasmas* **27**, 082305 (2020).
13. *Electromagnetic modeling of parametric instability for slow waves in lower hybrid frequency range*, J. Bao, Z. Lin, W. L. Zhang, and D. Li, *AIP Conference Proceedings* **2254**, 080003 (2020).
14. *Linear gyrokinetic simulations of reversed shear Alfvén eigenmodes and ion temperature gradient modes in DIII-D tokamak*, Hongyu Wang, Pengfei Liu, Zhihong Lin, and Wenlu Zhang, *Plasma Sci. Technol.* **23**, 015101 (2021).
15. *Gyrokinetic simulation of low-frequency Alfvénic modes in DIII-D tokamak*, G. J. Choi, P. Liu, X. S. Wei, J. H. Nicolau, G. Dong, W. L. Zhang, Z. Lin, W. W. Heidbrink and T.S. Hahm, *Nuclear Fusion* **61**, 066007 (2021).
16. *Global gyrokinetic simulation of neoclassical ambipolar electric field and its effects on microturbulence in W7-X stellarator*, J. Y. Fu, J. H. Nicolau, P. F. Liu, X. S. Wei, Y. Xiao, and Z. Lin, *Phys. Plasmas* **28**, 062309 (2021).
17. *Interpretation of electromagnetic modes in the sub-TAE frequency range in JET plasmas with elevated monotonic q-profiles*, N. Fil, S.E. Sharapov, M. Fitzgerald, G.J. Choi, Z. Lin, R.A. Tinguely, H.J.C. Oliver, K.G. McClements, P.G. Puglia, R.J. Dumont, M. Porkolab, J. Mailloux, E. Joffirin, and JET Contributors, *Phys. Plasmas* **28**, 102511 (2021).
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20. *Deep learning based surrogate models for first-principles global simulations of fusion plasmas*, G. Dong, X. Wei, J. Bao, G. Brochard, Z. Lin, W. Tang, *Nuclear Fusion* **61**, 126061 (2021).
21. *Role of wave-particle resonance in turbulent transport in toroidal plasmas*, G. Dong and Z. Lin, *Plasma Phys. Contr. Fusion* **64**, 035005 (2022).
22. *Verification and validation of gyrokinetic and kinetic-MHD simulations for internal kink instability in DIII-D tokamak*, G. Brochard, J. Bao, C. Liu, N. Gorelenkov, G. Choi, G. Dong, P. Liu, J. Mc.Clenaghan, J. H. Nicolau, F. Wang, W. H. Wang, X. Wei, W. L. Zhang, W. Heidbrink, J. P. Graves, Z. Lin, H. Lutjens, *Nuclear Fusion* **62**, 036021 (2022).
23. *Regulation of Alfven eigenmodes by microturbulence in fusion plasmas*, P. Liu, X. Wei, Z. Lin, G. Brochard, G.J. Choi, W.W. Heidbrink, J.H. Nicolau, and G. R. McKee, *Phys. Rev. Lett.* **128**, 185001 (2022).
24. *Verification of a fully kinetic ion model for electromagnetic simulations of high-frequency waves in toroidal geometry*, Y. Y. Yu, X. S. Wei, P. F. Liu, and Z. Lin, *Phys. Plasmas* **29**, 073902 (2022).
25. *Global gyrokinetic simulations of electrostatic microturbulent transport using kinetic electrons in LHD stellarator*, Tajinder Singh, Javier H Nicolau, Zhihong Lin, Sarveshwar Sharma, Abhijit Sen, Animesh Kuley, *Nuclear Fusion* **62**, 126006 (2022).
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29. *Reconstruction of tokamak plasma safety factor profile using deep learning*, Xishuo Wei, Shuying Sun, William Tang, Zhihong Lin, Hongfei Du, Ge Dong, *Nuclear Fusion* **63**, 086020 (2023).
30. *Global gyrokinetic simulations of the impact of magnetic island on ion temperature gradient driven turbulence*, J. C. Li, J. Q. Xu, Y. R. Qu, Z. Lin, J. Q. Dong, X. D. Peng, J. Q. Li, *Nuclear Fusion* **63**, 096005 (2023).
31. *A new paradigm for fast and repetitive chirping of Alfvén eigenmodes*, Junyi Cheng, Wenlu Zhang, Zhihong Lin, Jian Bao, Chao Dong, Jintao Cao, and Ding Li, *Nuclear Fusion* **63**, 124004 (2023).
32. *Saturation of fishbone instability by self-generated zonal flows in tokamak plasmas*, G. Brochard, C. Liu, X. Wei, W. Heidbrink, Z. Lin, N. Gorelenkov, J. Bao, A. R. Polevoi, M. Schneider, S. H. Kim, S. D. Pinches, P. Liu, J. H. Nicolau, and H. Lutjens, *Phys. Rev. Lett.* **132**, 075101 (2024).
33. *Cross-scale Interaction between Microturbulence and Meso-scale Reversed Shear Alfvén Eigenmodes in DIII-D Plasmas*, P. Liu, X. Wei, Z. Lin, W. W Heidbrink, G. Brochard, G. J. Choi, J. H. Nicolau, and W. Zhang, *Nuclear Fusion* **64**, 076007 (2024).
34. *Effects of hydrogen isotope species on ITG microturbulence in LHD*, Y. Q. Qin, Y. C. Chen, G. Y. Sun, J. Nicolau, and Z. Lin, *Plasma Phys. Contr. Fusion* **66**, 085004 (2024).
35. *A gyrokinetic simulation model for 2D equilibrium potential in the scrape-off layer of a field-reversed configuration*, W. H. Wang, X. S. Wei, Z. Lin, C. Lau, S. Dettrick, T. Tajima, *Phys. Plasmas* **31**, 072507 (2024).
36. *Saturation of fishbone instability through zonal flows driven by energetic particle transport in tokamak plasmas*, G. Brochard, C. Liu, X. Wei, W. Heidbrink, Z. Lin, M.V. Falessi, F. Zonca, Z. Qiu, N. Gorelenkov, C. Chrystal, X. Du, J. Bao, A. R. Polevoi, M. Schneider, S. H. Kim, S. D. Pinches, P. Liu, J. H. Nicolau, H. Lutjens, and the ISEP group, *Nuclear Fusion* **65**, 016052 (2025).
37. *Transfer Learning Nonlinear Plasma Dynamic Transitions in Low Dimensional Embeddings via Deep Neural Networks*, Zhe Bai, Xishuo Wei, William Tang, Leonid Oliker, Zhihong Lin, Samuel Williams, *Machine Learning: Science and Technology* **6**, 025015 (2025).