GPS-TTBP:
Project Overview

P.H. DIAMOND, UCSD
PRINCIPAL INVESTIGATOR

OUTLINE

i.) Personnel

ii.) Organization

iii.) Scientific Program

iv.) Recent Activities and Recognition

v.) Near Term Plans

i.) PERSONNEL

- **P.H. Diamond, Principal Investigator, UCSD**
- **Fred L. Hinton, Senior Research Scientist, UCSD**

- Dr. John Mandrekas, DOE OFES - **Office of Science Program Officer**

Collaborating Institutions/P.I.'s
- Taik-Soo Hahm (institutional co-PI), Weixing Wang, Gregory Rewoldt, Stephane Ethier, PPPL
- Wendell Horton (institutional co-P.I.), Francois Waelbroeck, U TX*, Austin*
- Zhihong Lin (institutional co-PI), Liu Chen, Yong Xiao, Igor Holod, Wenlu Zhang, UCI
- Scott Klasky (institutional co-P.I.), *ORNL*
- Viktor Decyk (institutional co-P.I.), *UCLA*
- Kwan-Liu Ma (institutional co-P.I.), *UC Davis*
- Mary Hall (institutional co-P.I.), *USC*
- Mark Adams (institutional co-P.I.), *Columbia U*

Domestic Collaborators
- George Tynan, Ozgur Gurcan, Christopher Holland, Stefan Mueller, Christopher McDevitt (UCSD),
- C.S. Chang (*New York University*), Keith Burrell (*General Atomics*),
- Stanley Kaye, Daren Stotler (PPPL)

International Collaborators
- Jiaqi Dong, Jiangang Li (*China*) • Yanick Sarazin, Virginie Grandgirard (*France*)
- Sanae-I Itoh (*Japan*) • Gyung Su Lee, Hyeon Park (Korea)

Embedded Scientific Application Partnership (SAP):
Scientific Data Management Technologies to Accelerate Fusion Scientific Discovery
- Arie Shoshani (PI), *LBNL*

→ **GPS leverages off and collaborates with:**

- **base program at: PPPL, UCI, UCSD**
- **G.S.E.P. (Lin)**
- **C.P.E.S. (Chang)**

} **share 8M hr. INCITE Award with GPS**

→ **Postdocs Supported by GPS:**

- **Yong Xiao, UCI**
- **Igor Holod, UCI**
- **Wenlu Zhang, UCI**
- **Kazuhiro Miki, UCSD (to arrive 5/08)**
- **2 interviews pending, UCI, UCSD**

ii.) ORGANIZATION

→ **Executive Committee (monthly teleconference)**

P.H. Diamond, UCSD - P.I., Physics

Z. Lin, UCI - Computation

T.S. Hahm, PPPL - Physics

W. Wang, PPPL - Computation

Y. Xiao, UCI - GTC Code Development

S.Klaskly, ORNL
S.Ethier, PPPL } **- High Performance Computing**

S. Kaye, PPPL - Validation

G. Tynan, UCSD - Validation

→ **GPS Computing**

- **independent but interactive streams of code development and physics studies within:**

  GTC FRAMEWORK

- **West:** **Irvine, et al. (Lin)**

  GTC Code, etc.

  East: **PPPL, et al. (Wang)**

  GTC - S Code, etc.

→ **common:**

  physics program

  analysis tools

  supporting theory program

  supporting HPC program

GPS-TTBP Computing Resources

- ORNL Jaguar CPU hours: 3.7M (INCITE + Director)+4.5M (250TF pioneer application)
- NERSC Franklin MPP hours: 10M (~1.5M ORNL hours)
- TACC at U. Texas Lonestar & Ranger: ?

→ **Project Advisory Committee**

C.-S. Chang, C.I.M.S./N.Y.U. - Chair

X. Garbet, C.E.A., Cadarache

K.H. Burrell, G.A.

Y. Idomura, J.A.E.A.

T.-H. Watanabe, N.I.F.S.

M. Norman, U.C.S.D.

iii.) SCIENTIFIC PROGRAM

1.) Physics Studies in Drift Wave Turbulence and Transport

2.) GTC Framework Development

3.) High Performance Computing

4.) Validation of Gyrokinetic Models

1.) Physics Program

a.) Turbulent transport of toroidal momentum

- motivated by intrinsic rotation phenomena
- goal: understanding of off-diagonal toroidal momentum flux $\rightarrow$ pinch and residual stress
- special attention to:
  - relation of v_ϕ and *n* pinch
  - $\langle v_E \rangle'$ and neoclassical effects
  - anomalous momentum transport in electron channel-dominated regimes (i.e. NSTX)

b.) Collisionless Trapped Electron Mode (CTEM) Turbulence (Early Appl. Topic)

- motivated by electron thermal, particle transport
- goal: - understand saturation mechanisms and transport with strong resonance coherency
  - compare/contrast with ETG studies (ongoing at PPPL)
- special attention to:
  - zonal flow, corrugation effects
  - resonance detuning, distortion
  - CTEM turbulence spreading
  - related EPM avalanching (GSEP)

c.) Nonlocality in Turbulence and Transport

- motivated by ρ_* scaling, edge-core coupling

- goal: understand physics and mechanism of departure from quasi-local GB model

- special attention to:
  - ρ_* - ν_* interplay, via shear flows
  - testing models of spreading
  - edge - core spreading/coupling
  - physics model for turbulence intensity profile

d.) Secondary Structure Dynamics

- motivated by critical role of self-generated flows, structures in regulating turbulence, now universally acknowledged

- goal: elucidate detailed physics of flow structure, evolution, feedback-especially in collisionless regimes

- special attention to:
  - collisionless ZF saturation
  - spreading - ZF interaction
  - space-time flow structure
  - mean flow - zonal flow interplay

2.) GTC FRAMEWORK

GTC Physics Modules

UCI

- Perturbative (δf) method for ions
- Fluid-kinetic hybrid electron model for electrons
  - Collisionless trapped electron mode (CTEM) turbulence
  - Electromagnetic turbulence with kinetic electrons
  - Shear Alfven wave (SAW) excited by energetic particle
- Multi-species via OO Fortran
  - Energetic particle diffusion by microturbulence
- Guiding center Hamiltonian in magnetic coordinates
- Global field-aligned mesh: truly global geometry
- General geometry MHD equilibrium using cubic spline
- Fokker-Planck collision operators via Monte-Carlo method

GTS turbulence simulation capabilities for tokamak experiment

- Gyrokinetic Tokamak Simulation (GTS) code: generalized gyrokinetic particle simulation model
- Shaped cross-section; experimental profiles; consistent rotation and equilibrium $\mathbf{E} \times \mathbf{B}$ flow; linear Coulomb collisions; $\cdots$
- Interfaced with MHD equilibrium codes (based on ESI interface) and TRANSP data base
- Kinetic(electrostatic) electrons via the split-weight scheme
- Switches to control physics modules: ITG, ETG, kinetic electrons (TEM, ITG-TEM), ...
- Linear coupling with neoclassical simulation by GTC-NEO

Drift-kinetic PIC simulation of neoclassical transport

- GTC-NEO: δf global drift-kinetic PIC code
- Calculates neoclassical fluxes, E_r, E_θ, j_b, etc
- Nonlocal physics due to large ion orbits
- Two species now: ions + electrons
- Momentum, energy and particle number conserving collisions
- Interfaced with MHD equilibrium codes and TRANSP data base
- It is routinely applied to the analysis of NSTX discharges

GTC Plan

UCI

- Version integration & control (with *Decyk*)
- Physics modules
  - Full-f ion & profile evolution
  - GTC-XGC core-edge coupling (with CPES), turbulence-Alfven wave coupling (with GSEP), & turbulence-neoclassical coupling
- Particle noise analysis and control
  - Characterization of particle noise in full-f
  - Deterministic collision operator (with *Hinton*)
- Particle-field domain-decomposition for 100,000+ cores
- PIC optimization for multi-core (with *Hall* of PERI & *Wichmann* of Cray, *Either*)
- Visualization of particle-field interaction (with *Ma* of IUSV)
- Parallel I/O, data streaming, workflow, & dashboard (with *Klasky* of SDM)
- Synthetic diagnostics (with *Holland* & *Tynan*)

Short and long term plans for PPPL codes

- A web-based user interface is being developed
- full-f capability is being tested (with Kolesnikov and Lee)
- multi-ion species to be developed
- EM to be developed (with Lee and Startsev)
- multi-ion species into GTC-NEO with a new δf scheme and collision operator (with F. L. Hinton)
- integrated δf simulation capability with nonlinear interplay between neoclassical and turbulent dynamics

Advances in High Performance Computing for the GTC framework

Problem

- Run on more than 10K processors.
- Grids getting larger.
- 128-bit floating-point capabilities enable each processor to simultaneously execute up to four floating-point operations per core.
- Target more end-users.

Solution

- Replace current IO strategy with ADIOS and use particle domain decomposition.
- Use OpenMP + MPI.
- Vectorize key points in code to use SSE3 instruction set.
- Develop an easy to use analysis framework.

GPS-TTBP Workshop on GTC Framework Development

- UC Irvine, January 24, 2008
- 20 attendees from UCSD, UCI, UCLA, UCD, USC, U. Texas, PPPL, & ORNL
- Talks and discussions on project overview, GTC status & application, GTC framework development plan
- Near term action items
  - GTC CVS version for ORNL pioneer application (*Xiao*, done)
  - Version integration (*Decyk*)
  - I/O and Daskboard (*Klasky*)
  - Particle-field interaction & front tracking in CTEM (*Ma*)
  - Optimization for Jaguar (*Hall & Ethier*)
  - Parallelization for 100,000+ cores ?

4.) Validation of Gyrokinetic Models

→ definition: GPS-TTBP Workshop on Physics and Validation; UCSD: 2/29, 3/1

- Participants from PPPL, UCI, UCSD, Univ. TX, UCLA, G.A., NYU
- Mix of simulation, theory, experiment
- Intensive informal group discussion

→ Outcome:

- Validation focus:

  δf gyrokinetic models of ion thermal and particle flux with "dynamic edge boundary conditions"

$\rightarrow$ rationale:

$\rightarrow$ validation should follow "front" of physics studies

- off diagonals (pinch) important, so choice:
  - stresses χ_i; D and V
  - breaks flux $\leftrightarrow$ diffusion identity
  - n.b. caution: particle source ambiguous
- dynamic b.c. $\Rightarrow$ incorporate inward spreading from edge to boost intensity levels at $\rho > .6$!?

Other Issues:

- explore low-*n* modes (i.e. trapped ion) excluded in flux tube schemes
- validation metric should:
  - reward success with flux *and* fluctuations
  - account for noise?!
- need to quantitatively characterize profile stiffness

→ Outlook for GPS Validation Program

- GPS-TTBP validation effort will work closely with related DIII-D effort
- C. Holland and G. Tynan will help supervise postdocs working on validation
- Validation will require:

  - common, accessible toolkit for GTCF

  - report of noise monitoring
- Interviews for validation postdocs ongoing

→ Related Work: Tests of Physics Basics of Transport Models

→ Seeks to explore validity, self-consistency of standard modelling approximations (I.e. quasilinear theory)

→ Likely productive synergy with validation effort

iv.) Recent Activities and Recognition

a.) Activities

→ Two “Kick-Off Workshops”:

a.) GTC Framework - UCI, 1/24

b.) Physics and Validation - UCSD, 2/29-3/1

→ Project Meeting at TTF: 3/28

b.) Achievements

→ INCITE Award (joint with GSEP, CPES)

→ 3 U.S. IAEA Selections:

P.H. Diamond, et al. - Toroidal Momentum Transport Physics

Z. Lin, et al. - Physics Basis Of Transport Models

W. Wang, et al. - Turbulence ↔ Neoclassical Interaction

v.) Future Plans

a.) Near-term emphasis on:

- toroidal momentum transport, including $\langle V_E \rangle'$ and neoclassical effects/feedback
- CTEM physics
- initial validation studies

b.) Activities:

- PSACI PAC
- meeting with International members of Project PAC at EPS, IAEA
- all hands meeting at APS
- possible small informal working meetings
  i.e. possible topic: secondary structures, flows and multi-scale interaction