E-Infrastructures

H2020-EINFRA-2015-1

EINFRA-5-2015: Centres of Excellence for computing applications

EoCoE

Energy oriented Center of Excellence for computing applications

Grant Agreement Number: EINFRA-676629

D5.4 M36

Towards the coupling of gyrokinetic and fluid codes

Project and Deliverable Information Sheet

EoCoE	Project Ref:	EINFRA-676629
	Project Title:	Energy oriented Centre of Excellence
	Project Web Site:	http://www.eocoe.eu
	Deliverable ID:	D5.4 M36
	Lead Beneficiary:	MPG
	Contact:	Eric Sonnendrücker
	Contact's e-mail:	sonnen@ipp.mpg.de
	Deliverable Nature:	Report
	Dissemination Level:	PU*
	Contractual Date of Delivery:	M36 30/09/2018
	Actual Date of Delivery:	M36 21/09/2018
	EC Project Officer:	Carlos Morais-Pires

* - The dissemination level are indicated as follows: PU – Public, CO – Confidential, only for members of the consortium (including the Commission Services) CL – Classified, as referred to in Commission Decision 2991/844/EC.

Document Control Sheet

Document	Title :	Towards the coupling of gyrokinetic and fluid codes
	ID :	D5.4 M36
	Available at:	http://www.eocoe.eu
	Software tool:	LaTeX
Authorship	Written by:	Stefan Possanner, Eric Sonnendrücker
	Contributors:	Stefan Possanner, Asad Ali, Florian Holderied, Xin Wang, Eric Sonnendrücker, Alexey Mishchenko, Natalia Tronko
	Reviewed by:	E. Audit, N. Girard, PEC members

Contents

List of Figures

1. Optimized filtering of particles in the velocity space. Implementation and tests in gyrokinetic Particle In Cell Codes

The aim here was on the one hand to reduce the needed resolution in a gyrokinetic code by using a reduced description by a fluid code in regions of the physical space where this is possible and on the other hand to reduce the noise in PIC codes by using noiseless fluid data as a control variate. However it proved to be quite difficult in the core of the Tokamak that is for the moment the only part simulated by our gyrokinetic codes to improve on a control variate given by the initial Maxwellian to which the distribution function remains quite close within the whole simulation. We thus left this issue for more academic situations shown in the next section. This will be more useful in production codes when those will be extended towards the edge of the plasma and the scrape-off layer.

Instead, we developed a mixed variable formulation of electromagnetic gyrokinetics that was able in general electromagnetic simulations in the core of the Tokamak plasma as well to reduce the noise in PIC codes as well as to use larger time steps and eliminate the cancellation problem that has plagued electromagnetic PIC simulations for many years. This has been implemented in the PIC codes GYGLES and ORB5 and will also be implemented in the future electromagnetic version of GYSELA.

The idea was first developed in [6, 5] for problems close to the MHD limit, with the idea to decompose the parallel vector potential $A_\|$ into a part that compensates exactly the contribution from the parallel gradient of the scalar potential, and is calculated from it and the rest. This enabled the term causing the cancellation problem in the equation for $A_\|$ to remain small and so avoid the cancellation problem close to the MHD limit.

Within the EoCoE project, we could extend this idea to the general case, by setting back the decomposition at each time step, so that the term causing the cancellation remains small in all cases during the simulation as it restarts from 0 at each time step. This can be interpreted as an integrating factor method. This was developed in the papers [3, 4]. Another paper in preparation [9], is developing the theoretical framework for this new model. On the other hand a hamiltonian framework compatible with the implementation of the codes has been developed for verification purposes [10, 11].

2. Coupling of reduced kinetic and fluid codes within the SELALIB framework

The coupling between solvers for reduced kinetic equations and fluid solvers has been addressed in three separate topics:

1. Heterogeneous multiscale methods: heat flux computation in a dynamical plasma background
2. Energetic particle effects on cold electrons: finite element based PIC code coupled to cold plasma model
3. Kinetic-MHD hybrid modeling: energy-conserving current-coupling schemes

Methodologies and results for the respective topic are presented in the following subsections. In the first topic, heterogeneous multiscale methods (HMM), we studied the coupling between the Vlasov-Poisson system and the corresponding moment equations for mass, momentum and energy. This is a prototypical system for developing HMM algorithms, where different model equations and different numerical methods are used for different problem scales. We developed a self-consistent scheme for a finite difference based PIC solver for the Vlasov-Poisson system coupled to a high-order, essentially non-oscillatory (ENO) finite volume scheme for the moment equations. The obtained results are a first building block towards HMM algorithms designed for an efficient study of plasma kinetic turbulence in a self-consistent, dynamical background.

With regard to the second topic, energetic particles (EPs), we were interested in a particular kinetic-fluid hybrid model for high-frequency phenomena, i.e. for frequencies higher than the ion plasma frequency. The model describes a cold population of bulk electrons in terms of a linearized momentum conservation law and assumes a static ion background. The total plasma current is composed of the bulk electron current and a "hot" portion coming from EPs, which are described by a Vlasov equation. The current coupling takes effect as a source in Ampère's law, which is solved alongside Faraday's law for the magnetic field evolution. A spline based finite element code has been developed for this system, coupled to a PIC solver for the Vlasov equation describing the EPs. The new hybrid code has been verified by means of one-dimensional (1D) test problems with particular attention to the growth and ensuing saturation of unstable modes.

In the third topic, kinetic-MHD hybrid modeling, our goal was to develop a hybrid code that enables the simulation of EP effects on MHD (magneto-hydro-dynamic) stability. The code should allow for the study of non-linear saturation and long-time dynamics of such a system. Therefore, our focus was on the exact conservation of dynamical invariants, in particular the total energy. The first step was to establish an energy-conserving framework for model reduction, which allows for the consistent derivation of a reduced kinetic-MHD hybrid model from first principles. On the kinetic level, we developed the technique of "variational averaging" (VA), which is a simplified version of the well-known Lie-transform approach. In case of a non-uniform, time-dependent background magnetic field, VA allowed us to derive a drift-kinetic equation that is consistent with the ordering assumptions for MHD equations. Moreover, we developed a new current coupling scheme for the drift-kinetic-MHD system which satisfies an exact energy theorem. In order to sustain exact energy conservation on the discrete level, the discretisation of the new current coupling scheme with techniques from finite element exterior calculus (FEEC) is ongoing. Code verification is based on the system's dispersion relation, which has been solved numerically.

2.1 Heterogeneous multiscale methods: heat flux computation in PIC codes

As a first step towards heterogeneous multiscale methods (HMM) for plasma kinetic turbulence, we studied the Vlasov-Poisson system coupled to its moment equations for mass, momentum and energy. In future HMM, the moment equations can play the role of the macro scale model, solved on a coarse mesh, wheres the Vlasov-Poisson system plays the role of the micro model providing the closure relations. At the center of this work was the accurate and efficient computation of the heat flux from Lagrangian marker distributions. We developed high-order schemes for the kinetic-fluid hybrid system in one spatial dimension (1D1V), where the kinetic part is solved with a particle-in-cell (PIC) Monte-Carlo method, while the fluid part is solved with a high-order, essentially-non-oscillatory (ENO) finite volume scheme. The fluid moments were used to construct a control variate for the Monte-Carlo integration of the heat flux. This lead to considerable variance reduction in case that the distribution function is not too far from a Maxwellian distribution (Gaussian in velocity). In this way, we were able to describe kinetic plasma perturbations (δf-method) in a self-consistent, dynamical background computed from the moment equations.

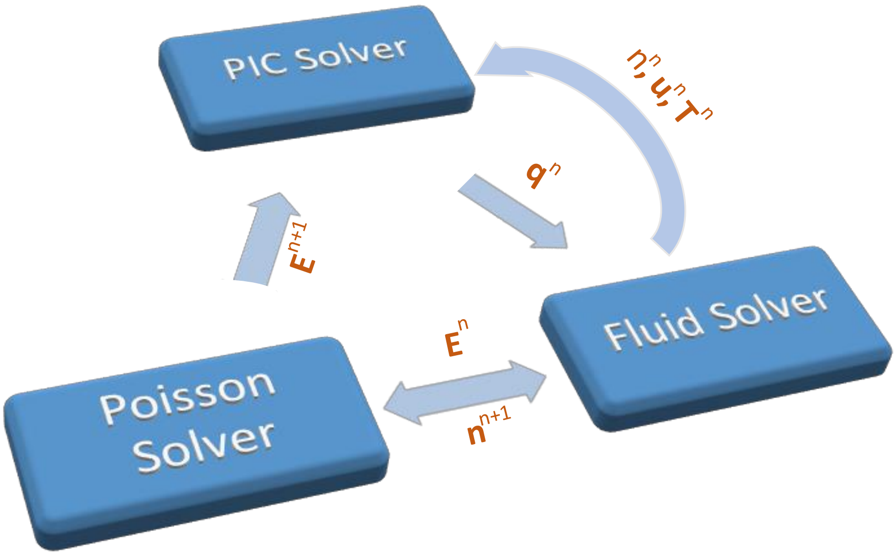

Figure 1: Coupling strategy for the kinetic-fluid Vlasov-Poisson hybrid scheme: q^n denotes the heat flux, E^n stands for the electric field and n^n, u^n and T^n are the fluid variables density, velocity and temperature, respectively, after n time steps.

The velocity moments of the Vlasov equation lead to the Euler equations in conservative form, augmented by an acceleration due to the electric field and by the heat flux. For the Euler equations we implemented finite volume methods with different order ENO reconstruction from the cell averages: zeroth order (Rusanov), first order (MUSCL) and up to fourth order polynomials. Runge-Kutta methods of corresponding order were used for time stepping. As the particle pusher in the PIC code we used the symplectic Verlet scheme. The control variate was constructed from the local Maxwellian defined by the solution of the moment equations. Due to the finite volume discretisation, the heat flux was needed at the cell interfaces, which were thus chosen as the space grid for the Poisson solver and for particle smoothing in the PIC code. The smoothing and the computation of the electric field at the marker positions was done with third order B-splines. One of the kinetic-fluid coupling strategies investigated in this work is illustrated in Fig. 1. It involves the following steps:

1. The Fluid solver passes the current instances of the density n^n (n as a superscript denotes the nth time step), the velocity u^n and the temperature T^n to the PIC solver. The PIC solver uses this information to construct a control variate from the local Maxwellian defined by these fluid variables.

2. Using the control variate, the PIC solver performs an efficient computation of the heat flux q^n at the cell interfaces from the current marker positions in phase space.

3. The heat flux q^n and the electric field E^n (from the Poisson solver) are passed to the fluid solver, which is then run to update the fluid variables.

4. The new density n^{n+1} is passed to the Poisson solver for the computation of the

new electric field E^{n+1}, which is then used to push the particles.

In practice this algorithm is implemented in combination with the Verlet scheme for particle pushing. It is thus more complicated because of the multiple steps in the Verlet scheme, but the concept remains the same. The different components of the hybrid code have been verified systematically in the linear regime. Fourth order convergence has been achieved for the fluid solver. The PIC solver with dynamical control variate was verified for Landau damping, two-stream and bump-on-tail initial instabilities. Heat flux computations with reduced variance due to the dynamical control variate were successful. However, further work is needed to improve the control variate in the non-linear phase.

Methodology and results can be found in [1].

2.2 Energetic particle effects on cold electrons

In this work we considered the coupling between a fluid model for cold electrons and the electromagnetic Vlasov equation for energetic particles (EPs). The coupling was via Ampère's law, where the total current density is the sum of fluid and EP contributions. This is called a current coupling scheme. In the high-frequency regime, i.e. with mode frequencies much larger than the ion plasma frequency, EPs can drive unstable modes and thus lead to non-linear physics evolving on long time scales. We computed the dispersion relation of the hybrid scheme for the case of a homogeneous equilibrium with uniform magnetic background. The dispersion relation was solved numerically with a Newton method. We obtained the classical result for cold electrons, augmented by a correction term due to the EPs, which features non-zero imaginary part (damped and growing modes). It was found that instabilities occur only for anisotropic (in temperature) Maxwellians.

As a next step we developed a kinetic-fluid hybrid scheme based on third order B-spline finite elements for the Maxwell equations and based on a particle-in-cell (PIC) solver for the Vlasov part. Variations in one space dimension (1D) were considered, which corresponds to modes that propagate along the background magnetic field. The linearized momentum equation for the bulk current density could be solved analytically. For time stepping in Maxwell's equations we used an implicit Crank-Nicolson scheme. The PIC solver was implemented with a control variate method for variance reduction in order to compute the EP current efficiently. A Boris scheme was used to push the particles.

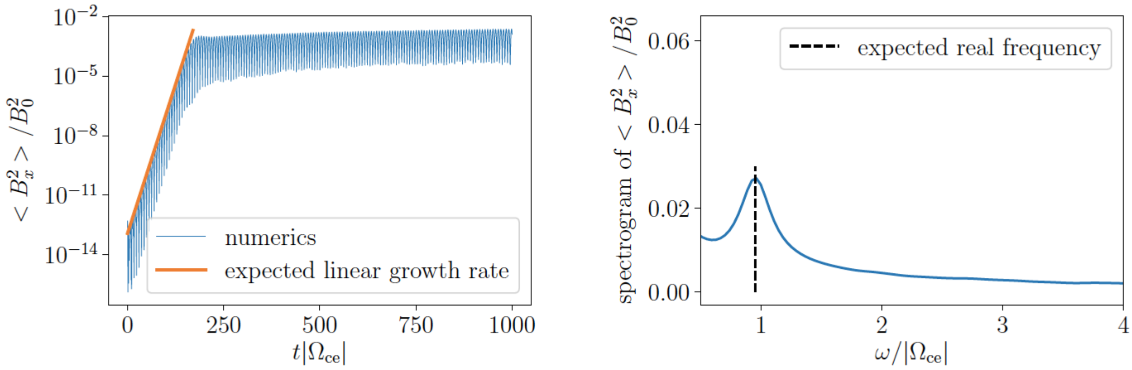

Figure 2: Verification test for the current coupling hybrid scheme: mode growth and saturation (left panel) and mode frequency (right panel). B_x stands for the x-component of the magnetic field perturbation and Ω_{ce} denotes the electron cyclotron frequency.

The new scheme was verified in the linear regime by means of the previously solved dispersion relation. The growing modes (instabilities) have been studied in particular. Fig. 2 displays the typical results from a verification test. The normalized quadratic magnetic field in x-direction is considered. The left panel shows a comparison between the simulated growth (and saturation) of the mode and the growth rate computed from the dispersion relation. The left panel depicts the mode spectrum, where the maximum coincides well with the analytical value.

The test cases considered thus far did not feature longitudinal magnetic waves, hence $\nabla \cdot \mathbf{B} = 0$ was satisfied automatically. In order to treat also longitudinal perturbations, the implementation of Maxwell's equations based on finite element spaces of the de Rham complex is ongoing. This should guarantee improved long time stability for non-linear simulations.

Methodology and results are currently being compounded in [2].

2.3 Kinetic-MHD hybrid modeling

This work was concerned with the derivation and implementation of an energy conserving drift-kinetic-MHD hybrid model, adapted to physical scenarios in strongly magnetized fusion plasmas. To guarantee consistency, our goal was to derive the reduced kinetic and MHD models in one unified framework. This is in contrast to usual approaches, where existing drift-kinetic equations have been coupled to the standard MHD equations in adhoc fashion. We adopted the current coupling approach, in which the charge density and the current density, composed of bulk (MHD) and energetic (drift-kinetic) contributions, account for the coupling. The starting equations were the two-fluid Braginskii equations for the bulk and the six-dimensional (3D3V) Vlasov equation for the energetic particles (EPs), coupled via Maxwell's equations for the electromagnetic fields. A common set of ordering assumptions was imposed on both systems and the model reduction was then carried out in a consistent way via truncation at the appropriate order of approximation. The total energy of the reduced systems was conserved in our approach. A novel, extended drift-kinetic-MHD current coupling scheme could be derived, which is suited for tokamak and stellarator plasmas. We present some details of our method in the subsequent paragraphs. The derived hybrid model was then used as the basis for an energy-conserving numerical scheme based on finite element (for MHD) and particle-in-cell (for drift-kinetics) methods. The implementation of this scheme is still ongoing.

With regard to the reduction of the 3D3V Vlasov equation to the 3D1V drift-kinetic equation, we developed a new method called "variational averaging" (VA). In contrast to the usual approaches, this method does not rely on Lie-transforms and is simpler form a mathematical point of view. VA enables the model reduction in non-homogeneous, time dependent magnetic backgrounds, which makes it particularly suitable for the coupling to MHD. Moreover, it preserves the Hamiltonian structure of the particle dynamics, thus yielding energy conservation automatically. We developed the mathematical theory of VA by proving the existence of the coordinate transformation leading to the dimensional reduction and by computing an error estimate for the reduced dynamics. The methodology of VA was then applied in the derivation of the new drift-kinetic-MHD hybrid scheme.

For the fluid part we followed the conventional reduction from the two-fluid Braginskii-Maxwell equations to the MHD equations, albeit under slightly different ordering assumptions. In particular, the current density need not be small in our model. This led to the derivation of "extended" MHD equations, featuring both the electron and the ion pressure rather than just one total pressure. Moreover, compared to standard MHD, the electric field has additional terms stemming from the ion inertia, which need to be kept for energy conservation. The coupling to the kinetic model was incorporated in the MHD derivation, such that we were able to prove energy conservation of the hybrid model at different orders of truncation. We computed the dispersion relations for the new hybrid models in order to identify the unstable modes originating from the EPs. These modes will be used for our scheme's verification in the future.

Methodology and results can be found or are currently being compounded in [7, 8].

References

[1] A. Ali. Hybrid algorithm for the vlasov-poisson system. Master's thesis, Technical University Munich, Garching, Germany, February 2018. Computational Science and Engineering.

[2] Florian Holderied. Hybrid modeling of whistler wave instability. Master's thesis, Technical University Munich, Garching, Germany, 2018. ongoing.

[3] R Kleiber, R Hatzky, A Könies, A Mishchenko, and E Sonnendrücker. An explicit large time step particle-in-cell scheme for nonlinear gyrokinetic simulations in the electromagnetic regime. *Phys. Plasmas*, 23:032501+12, 2016.

[4] A Mishchenko, A Bottino, R Hatzky, E Sonnendrücker, R Kleiber, and A Könies. Mitigation of the cancellation problem in the gyrokinetic particle-in-cell simulations of global electromagnetic modes. *Phys. Plasmas*, 24:081206+6, 2017.

[5] A Mishchenko, M Cole, R Kleiber, and A Könies. New variables for gyrokinetic electromagnetic simulation. *Phys. Plasmas*, 21:052113+6, 2014.

[6] A Mishchenko, A Könies, R Kleiber, and M Cole. Pullback transformation in gyrokinetic electromagnetic simulations. *Phys. Plasmas*, 21:092110+8, 2014.

[7] S. Possanner and X. Wang. Current coupling scheme for reduced kinetic/hydrodynamic models in strongly-magnetized plasmas with large currents. In preparation, 2018.

[8] Stefan Possanner. Gyrokinetics from variational averaging: Existence and error bounds. *J. Math. Phys.*, 59, 2018.

[9] E. Sonnendrücker, A Mishchenko, and N. Tronko. Lagrangian variational principle for the mixed-variable representation of electromagnetic gyrokinetic theory. In preparation, 2018.

[10] N. Tronko, A. Bottino, C. Chandre, and E. Sonnendrücker. Hierarchy of second order gyrokinetic Hamiltonian models for Particle-In-Cell codes. *Plasma Physics and Controlled Fusion*, 59:064008, 2017.

[11] N. Tronko, T. Bottino, A. Goerler, E. Sonnendrücker, D. Told, and L. Villard. Verification of gyrokinetic codes: theoretical background and applications. *Physics of Plasmas*, 24:056115, 2017.