

High Performance Computing in plasma physics and magnetic fusion

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Outline

Tokamak and stellarator physics

- Turbulence and transport: kinetic

- Large scale instabilities: MHD

- Plasma wave interaction in tokamaks: Maxwell

HPC in the european Fusion community

MHD simulations

- Finite Elements: the Jorek Code

- Efficient DG code for MHD

Gyrokinetic and kinetic models

- Derivation of gyrokinetic model

- From the continuous to the discrete action: FEM-PIC

- Field aligned semi-Lagrangian method

- Efficient 6D Vlasov solvers

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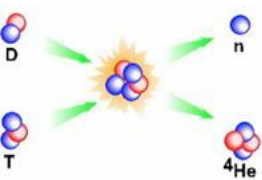
Derivation of gyrokinetic model

From the continuous to the discrete action: FEM-PIC

Field aligned semi-Lagrangian method

Efficient 6D Vlasov solvers

Controlled thermonuclear fusion



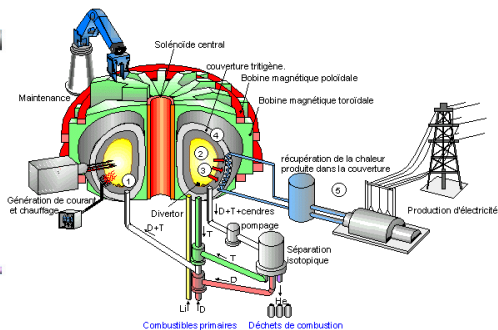
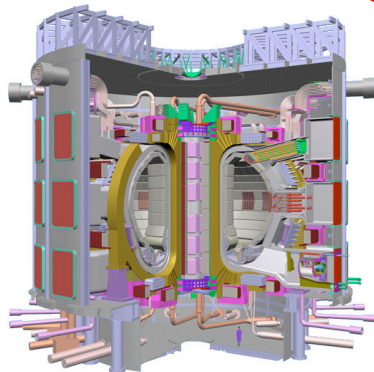
- ▶ Fusion conditions:
 $nT\tau_E$ large enough.
- ▶ $T \approx 100$ million $^{\circ}\text{C}$
fully ionized gas=plasma.



- ▶ Magnetic confinement (ITER)
- ▶ Inertial confinement
 - ▶ by laser (LMJ, NIF)
 - ▶ by heavy ions

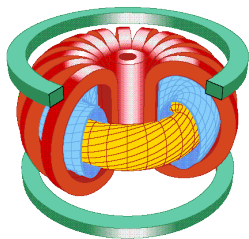
The ITER project

International project involving European Union, China, India, Japan, South Korea, Russia and United States aiming to **prove that magnetic fusion is viable source for energy.**

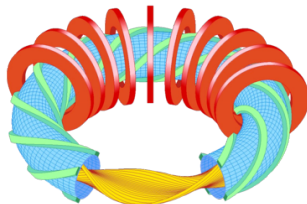


Two devices for magnetic fusion: tokamaks and stellarators

Tokamak



Stellarator



Modelling of Tokamak plasmas

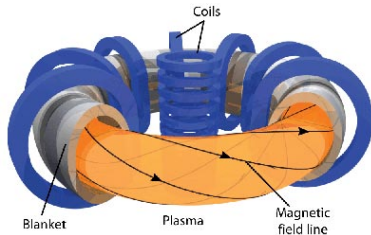
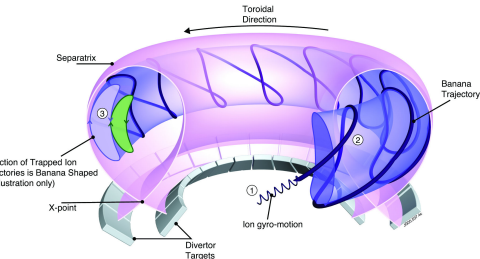
- ▶ A plasma is a collection of different species of charged particles.
- ▶ Basic model is Newton's law with pairwise interaction between particles which is largely dominated by electromagnetic force. Too many particles $n \approx 10^{19} m^{-3}$, numerically intractable.
- ▶ First reduced model: Kinetic Vlasov-Maxwell (+Landau collisions)
- ▶ Second reduced model: multi-fluid Euler-Maxwell
- ▶ Third reduced model: single fluid MHD
- ▶ Other reduced model: Maxwell's equation with dielectric tensor representing plasma

Kinetic models: Turbulent transport

- ▶ Plasma not very collisional and far from fluid state
 \Rightarrow Kinetic description necessary for shorter time scales. Fluid and kinetic simulations of turbulent transport yield very different results.
- ▶ Vlasov (6D phase space) coupled to 3D Maxwell

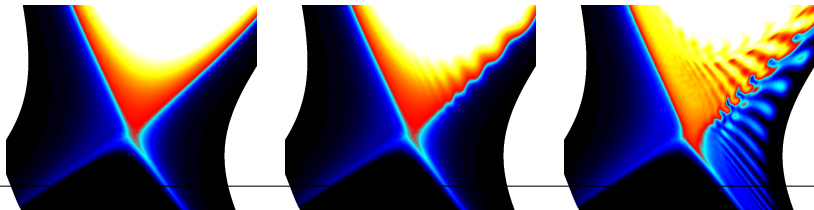
$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f = 0.$$

- ▶ Toroidal geometry



MHD: ELM

- ▶ In the tokamak **large scale instabilities** can appear in the plasma.
- ▶ The simulation of these instabilities is an **important subject** for ITER.
- ▶ Example of Instabilities in the tokamak :
 - ▶ **Disruptions**: Violent instabilities which can critically damage the Tokamak.
 - ▶ **Edge Localized Modes (ELM)**: Periodic edge instabilities which can damage the Tokamak.
- ▶ These instabilities are linked to the **very large gradient of pressure and very large current** at the edge.
- ▶ Many aspects of these instabilities are described by **fluid models** (MHD resistive and diamagnetic or extended)



Two-fluid model

- ▶ Computing the moments of the Vlasov equation we obtain the following two fluid model

$$\partial_t n_s + \nabla_x \cdot (m_s n_s \mathbf{u}_s) = 0,$$

$$\partial_t (m_s n_s \mathbf{u}_s) + \nabla_x \cdot (m_s n_s \mathbf{u}_s \otimes \mathbf{u}_s) + \nabla_x p_s + \nabla_x \cdot \overline{\overline{\mathbf{p}}}_s = \sigma_s \mathbf{E} + \mathbf{J}_s \times \mathbf{B},$$

$$\partial_t (m_s n_s \epsilon_s) + \nabla_x \cdot (m_s n_s \mathbf{u}_s \epsilon_s + p_s \mathbf{u}_s) + \nabla_x \cdot (\overline{\overline{\mathbf{p}}}_s \cdot \mathbf{u}_s + \mathbf{q}_s) = \sigma_s \mathbf{E} \cdot \mathbf{u}_s,$$

- ▶ coupled with Maxwell's equations

$$\frac{1}{c^2} \partial_t \mathbf{E} - \nabla \times \mathbf{B} = -\mu_0 \mathbf{J},$$

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0,$$

$$\nabla \cdot \mathbf{B} = 0, \quad \nabla \cdot \mathbf{E} = \frac{\sigma}{\epsilon_0}.$$

- ▶ $n_s = \int_{\mathbb{R}^3} f_s d\mathbf{v}$ the particle number, $m_s n_s \mathbf{u}_s = \int_{\mathbb{R}^3} m_s \mathbf{v} f_s d\mathbf{v}$ the momentum, ϵ_s the total energy and $\rho_s = m_s n_s$ the density.
- ▶ Isotropic pressures are p_s , stress tensors $\overline{\overline{\mathbf{p}}}_s$ and heat fluxes \mathbf{q}_s .

MHD: assumptions and generalized Ohm's law

- ▶ **quasi neutrality assumption:** $n_i = n_e \implies \rho \approx m_i n_i + O\left(\frac{m_e}{m_i}\right)$,
 $\mathbf{u} \approx \mathbf{u}_i + O\left(\frac{m_e}{m_i}\right)$
- ▶ **Magneto-static assumption :** $\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + O\left(\frac{V_0}{c}\right)$.
- ▶ We define $\rho = \rho_i + \rho_e$ and $\mathbf{u} = \frac{\rho_i \mathbf{u}_i + \rho_e \mathbf{u}_e}{\rho}$.
- ▶ Consequence of the quasi-neutrality:

$$\mathbf{u}_e = \mathbf{u} - \frac{m_i}{e\rho} \mathbf{J} + O\left(\frac{m_e}{m_i}\right)$$

- ▶ Summing the mass and moment equation for the two species we obtain:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{J} \times \mathbf{B} - \nabla \cdot \bar{\mathbf{p}} + O\left(\frac{m_e}{m_i}\right)$$

- ▶ For the pressure equation, we replace the **electronic velocity** by **full velocity** using the previous relation.

Extended MHD: model

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{J} \times \mathbf{B} - \nabla \cdot \bar{\bar{\mathbf{n}}},$$

$$\frac{1}{\gamma-1} \partial_t p_i + \frac{1}{\gamma-1} \mathbf{u} \cdot \nabla p_i + \frac{\gamma}{\gamma-1} p_i \nabla \cdot \mathbf{u} + \nabla \cdot \mathbf{q}_i = -\bar{\bar{\mathbf{n}}}_i : \nabla \mathbf{u},$$

$$\frac{1}{\gamma-1} \partial_t p_e + \frac{1}{\gamma-1} \mathbf{u} \cdot \nabla p_e + \frac{\gamma}{\gamma-1} p_e \nabla \cdot \mathbf{u} + \nabla \cdot \mathbf{q}_e = \frac{1}{\gamma-1} \frac{m_i}{e\rho} \mathbf{J} \cdot \left(\nabla p_e - \gamma p_e \frac{\nabla \rho}{\rho} \right) - \bar{\bar{\mathbf{n}}}_e : \nabla \mathbf{u} + \bar{\bar{\mathbf{n}}}_e : \nabla \left(\frac{m_i}{e\rho} \mathbf{J} \right) + \eta |\mathbf{J}|^2,$$

$$\partial_t \mathbf{B} = -\nabla \times \left(-\mathbf{u} \times \mathbf{B} + \eta \mathbf{J} - \frac{m_i}{\rho e} \nabla \cdot \bar{\bar{\mathbf{n}}}_e - \frac{m_i}{\rho e} \nabla p_e + \frac{m_i}{\rho e} (\mathbf{J} \times \mathbf{B}) \right),$$

$$\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{B} = \mathbf{J}.$$

- ▶ **Remark:** We can write easily the equation on the total pressure $p_e + p_i$. Possible simplification $p_e = p/2$.
- ▶ In Black: ideal MHD. In Black and blue: Viscous-resistive MHD. All the terms: Extended MHD.

Microwave beams in plasmas

- ▶ RF waves are typically used in magnetic fusion plasmas for
 - ▶ **Heating**: wave energy is transferred to particle motion exploiting the wave-particle resonances in a plasma, selectively heating electrons or ions
 - ▶ **Current drive**: transfer momentum to plasma in order to induce toroidal current to generate poloidal confinement field.
 - ▶ **Diagnostics**: temperature and density of a plasma can be determined by probing the plasma with RF waves
- ▶ Standard computations are based on short-wavelength asymptotics (ray tracing, beam tracing, ...).
- ▶ Such methods fail in some cases. So called **full-wave** solvers are then the model of choice.

Full-wave solvers

- ▶ Full-wave means Direct numerical solution of Maxwell's equations (including the “full” range of wavelengths).
- ▶ Popular approach: Finite Difference Time Domain (Yee's scheme) augmented with one equation for the induced current density J ,

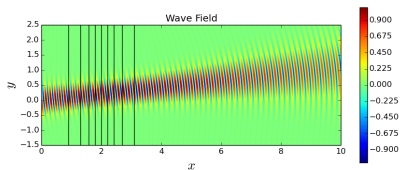
$$\begin{cases} \partial_t E - c \nabla \times B + \omega_p F = 0, \\ \partial_t B + c \nabla \times E = 0, \\ \partial_t F - \omega_p E - \omega_c \times F + \nu F = 0, \end{cases} \quad F = 4\pi J / \omega_p.$$

(For $\nu = 0$, this is a symmetric hyperbolic system; conserved energy.)

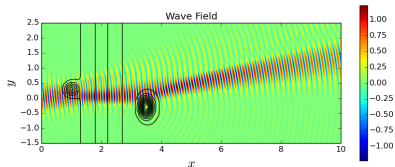
- ▶ Does not correctly take into account real geometry.
- ▶ New full wave solver based on [structure preserving finite elements](#) (FEEC: Arnold-Falk-Winther) under development.

Applications: Beam scattering by turbulence

- ▶ Turbulence at the edge of the plasma produces density blobs.
- ▶ Time-scale separation: We can consider blobs frozen in time.
- ▶ Each blob acts as a defocusing lens that can even split the beam:



A wave beam injected from the left boundary into a smooth density profile.

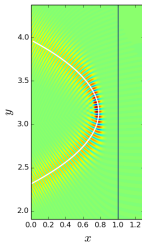


The same beam in presence of two density blobs.

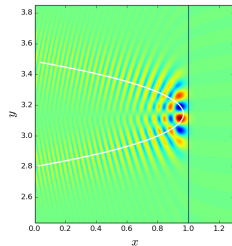
- ▶ Standard beam tracing techniques do not apply for such beams.

Applications: Reflectometry diagnostics

- ▶ Wave beams are reflected back when the electron density is sufficiently large (cut-off).
- ▶ From the phase shift of the reflected beam one obtains information on, e.g., the density profile.
- ▶ A fold caustic near the cut-off limits the applicability of ray and beam tracing methods:



refracted beam
(beam tracing applies)



reflected beam
(full-wave required)

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- ▶ European Fusion community organised within the [EUROfusion consortium](#) supported by EU
- ▶ Next to experimental devices HPC plays an important role: dedicated resources
 - ▶ HPC-FF (Germany): 2009-2013, 100 Tflops, 1080 nodes, 8-core Intel-Nehalem, 8640 cores. Part of JUROPA cluster at Jülich.
 - ▶ HELIOS (Japan): 2012-2016, 1.5 Petaflops, 4500 nodes, 16-core Intel SandyBridge, 72000 cores. Fully dedicated to fusion: 50% for Europe, 50% for Japan.
 - ▶ New machine in Italy available at end of this year. Will be part of bigger cluster at CINECA.

The High Level Support Team

- ▶ Main tasks for HLST

The HLST team is a **support unit** to ensure optimal exploitation of dedicated resources since 2009: HPC-FF, HELIOS, ...

- ▶ it is **not focused on its own academic research**.

- ▶ Support for code development

- ▶ Parallelise codes using e.g. OpenMP and/or MPI standards for massively parallel computers
- ▶ Improve the performance of existing parallel codes both at the single node and inter node levels
- ▶ Support the transfer of codes to new multiprocessors architectures
- ▶ Choose and if necessary adapt algorithms and/or mathematical library routines to improve applications for the targeted computer architectures

The NMPP division at IPP

- ▶ **Numerical Methods in Plasma Physics** division at Max-Planck Institute for Plasma Physics
- ▶ Develop **robust, verified and well-documented codes** for plasma physics and magnetic fusion.
- ▶ **From mathematical modeling to High Performance Computing**
- ▶ Models **derived rigorously from first principles** via asymptotic reduction: kinetic, gyrokinetic, fluid, MHD,
- ▶ Emphasis on well-posedness, energy principle, mathematical structure: **basis for verification tests**
- ▶ Discretisation adapted to features of model: **Structure preserving discretisation**
- ▶ **Single core efficiency** and **parallel scaling** important issues.

NMPP code suite

- ▶ Well written, tested and documented codes in **Fortran 2003**
- ▶ Can be used for testing new numerical concepts, learning, or as libraries for productions codes. Release versions expected this year.
- ▶ Collaborative development under Gitlab at MPCDF
- ▶ Major codes:
 - ▶ **SeLaLib**: Kinetic and gyrokinetic, Semi-Lagrangian and PIC (with Inria, U. Strasbourg, CNRS, CEA)
 - ▶ **Django-Jorek**: Finite Element code aimed at MHD (with Inria)
 - ▶ **Spiga**: Finite Element code based on Isogeometric analysis for Maxwell: coupled with particle tracker as a Full Orbit code, Full Wave code in frequency domain under development
 - ▶ **FEMilaro**: Finite Element code for fluid models (SOLPS)

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The JOREK code

- ▶ **Models:** reduced MHD models (reduction of the solution space) using potential formulation of the fields.
- ▶ **Physics in models:** two fluid and neoclassical effect, coupling with neutral ...
- ▶ Typical run of JOREK:
 - ▶ Computation of the **equilibrium** on a grid aligned to the magnetic surfaces.
 - ▶ Computation of the **MHD instabilities** perturbing the axisymmetric equilibrium.

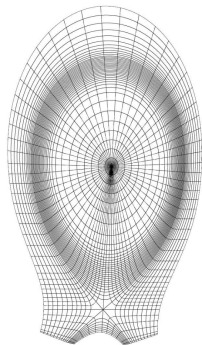


Figure: Aligned grid

Numerical methods

- ▶ **Spatial Discretization:** 2D Cubic Bezier finite elements + Fourier expansion.
- ▶ **Temporal discretization:** Implicit scheme + Gmres + Toroidal modes Block Jacobi preconditioning

New paths explored for MHD simulations

- ▶ JOREK code
 - ▶ Verification and non regression tests
 - ▶ Scaling issue with present algorithm:
 - ▶ **Preconditioner** for linear system **not efficient** for strongly non linear problems
 - ▶ New preconditioner with better properties has been derived and just being tested
 - ▶ **Matrix free implementation**, where jacobian matrix not explicitly computed, possible. This will **overcome the memory limitations**.
 - ▶ Simplified and modular version of numerical core of JOREK being developed for faster testing and evaluation of numerical algorithms.
- ▶ Evaluation of DG code FLEXI from Stuttgart for fusion applications.

Verification of the JOREK model

- ▶ The JOREK code implements different variants of reduced resistive MHD. *Stability issues observed in some situations.*
- ▶ A well posed model needs to enforce conservation or dissipation of total energy.
- ▶ Original model slightly modified so that the following energy theorem could be proved:

$$\frac{d}{dt} \int_{\Omega} \left(\frac{|\mathbf{B}|^2}{2} + \rho \frac{|\mathbf{v}|^2}{2} + \frac{1}{\gamma-1} p \right) = - \int_{\Omega} \eta(T) \frac{|\Delta^* \psi|^2}{R^2} - \int_{\Omega} \nu |\Delta_{\perp} u|^2$$

with $E = \frac{|\mathbf{B}|^2}{2} + \rho \frac{|\mathbf{v}|^2}{2} + \frac{1}{\gamma-1} p$ the total energy,
 $\mathbf{v} = -R \nabla u \times \mathbf{e}_{\phi} + v_{\parallel} \mathbf{B}$ and ψ the poloidal magnetic flux.

- ▶ Modified model has been implemented and indeed remains stable in situations where the original model is not.

Physics Based Preconditioner

- ▶ Present JOEREK preconditioner based on direct solver for each Fourier mode
- ▶ Exact for linear problems, but very inefficient in nonlinear case.
- ▶ Stiff problem due to hyperbolic structure with very different wave speeds
- ▶ Rewrite the hyperbolic system as a second order equation (well-conditioned): parabolization (L. Chacon).
- ▶ First tests on simpler problem exhibiting similar features.
- ▶ can be extended to the nonlinear hyperbolic system as MHD (and resistive MHD with additional splitting steps).

Damped waves problem

- ▶ We consider the damped wave problem

$$\begin{aligned}\frac{\partial p}{\partial t} + \frac{1}{\varepsilon} \nabla \cdot \mathbf{u} &= 0 \\ \frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\varepsilon} \nabla p &= -\frac{\sigma}{\varepsilon^2} \mathbf{u}\end{aligned}$$

with σ opacity, c light speed and $\varepsilon \approx \frac{1}{c} \approx \frac{1}{\sigma}$

- ▶ When $\varepsilon \rightarrow 0$ the model can be approximated by $\partial_t p - \nabla \cdot (\frac{1}{\sigma} \nabla p) = 0$.
- ▶ This problem is **stiff in time**. CFL condition is $\Delta t \leq C_1 \varepsilon h + C_2 \varepsilon^2$.
 \Rightarrow Use **implicit scheme** but the model is **ill-conditioned**
- ▶ Two reasons for the ill-conditioning:
 1. **the stiff terms** (which depend of ε)
 2. **the hyperbolic structure**.

Results with classical Solvers/Preconditioners

- ▶ Comparison between GMRES method with different preconditioning
- ▶ Jac (Jacobi), ILU (Incomplete LU), MG (Multigrid), SOR.
- ▶ Physics Based (PB)
- ▶ $\varepsilon_1 = 10^{-5}$ and $\varepsilon_2 = 10^{-10}$.

Mesh / solvers		Jac	ILU(0)	ILU(4)	MG(2)	SOR	PB
$4 \times 4, \varepsilon_1$	cv	✓	✓	✓	✓	✓	✓
	iter	27	11	1	38	8	1
	time	7.2 E-4	1.3E-3	7.7E-3	1.5E-2	1.4E-3	2.1E-3
$4 \times 4, \varepsilon_2$	cv	✓	✓	✓	✗	✓	✓
	iter	2.1E+4	11	1	-	8	1
	time	3.6E-1	1.3E-3	7.7E-3	-	1.5E-3	2.1E-3
$16 \times 16, \varepsilon_1$	cv	✓	✓	✓	✗	✓	✓
	iter	1.5E+4	18	9	140	20	1
	time	5.0E-0	2.3E-2	4.0E-1	5.0E-1	5.0E-2	2.1E-2
$16 \times 16, \varepsilon_2$	cv	✗	✓	✓	✗	✓	✓
	iter	-	18	9	-	20	1
	time	-	2.3E-2	4.0E-1	-	5.0E-2	2.1E-2
$64 \times 64, \varepsilon_2$	cv	✗	✗	✓	✗	✗	✗
	iter	-	-	632	-	-	1
	time	-	-	2.0E+1	-	-	4.2E-1

Results with the new Preconditioners

- Comparison between GMRES method with different Finite Elements. HB: Cubic Hermite-Bézier, BS(p) splines of degree p at $t = dt$ and $hdt = cst$

Mesh		HB	BS(3)	BS(4)	BS(5)
16 × 16	cv	✓	✓	✓	✓
	iter	3	2	1	1
	error	2.4E-11	7.7E-16	3.6E-11	1.5E-13
	time	0.38	4.14E-2	1.62E-2	2.1E-2
32 × 32	cv	✓	✓	✓	✓
	iter	6	2	1	1
	error	3.8E-13	5.8E-14	1.4E-13	5.2E-15
	time	14.08	0.18	5.5E-2	7.28E-2
64 × 64	cv	✓	✓	✓	✓
	iter	16	1	1	1
	error	4.3E-11	2.3E-12	8.8E-14	1.1E-13
	time	461.1	0.15	0.24	0.44

- The convergence tolerance is 10^{-10} and iter_max=100'000.
- The Preconditioner-solver tolerance is 10^{-7} for convergence and iter_max=1'000.

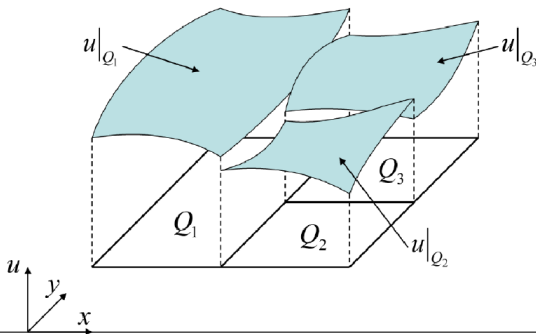
Comments on new preconditionner

- ▶ The good results for B-Splines (with maximum regularity) can be explained by the spectral properties of B-Splines discretized matrices,
- ▶ The global time can be improved by deriving appropriate preconditioners or solvers for the subsystems.
- ▶ The Generally Locally Toeplitz theory is a very good framework to study and improve the efficiency of a preconditioner
 - ▶ $H(\text{div}, \Omega)$ and $H(\text{curl}, \Omega)$ elliptic variational problems (needed for Maxwell, Stokes and some Physics-based subsystems)
 - ▶ Fast MultiGrid solver for elliptic problems (does not depend on the degree, nor the domain dimension)

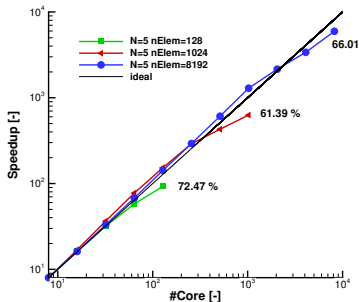
- ▶ FLEXI: Highly scalable explicit 3D DG-SEM solver, high order, unstructured hex-meshes for general conservation laws
- ▶ Resistive full MHD & anisotropic diffusion implemented and validated
- ▶ **Difficulties:** Find semi-implicit time integration maintaining scalability of the solver!
- ▶ Initialization: domain geometry, mesh and MHD equilibrium needed
- ▶ **Objectives:**
 - ▶ Assess DG versus JOEREK's FE for different fusion applications
 - ▶ Explore benefits of non conforming locally field aligned mesh which is easier to handle with DG, including in the vicinity of the separatrix.

Discontinuous Galerkin Method

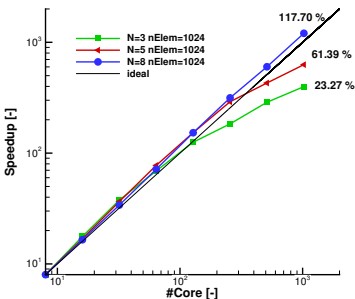
- ▶ From high order Finite Element Method (p-FEM):
Approximation solution is a **polynomial inside an element**
 - ▶ From Finite Volume (FV):
Riemann solvers to resolve **discontinuity at element interfaces**
- ⇒ **High order scheme**, low dissipation and dispersion errors
- ⇒ Allows **coarse unstructured meshes** for complex geometries
- ⇒ High potential for **parallel scaling** due to element local operators



Strong Scaling of FLEXI



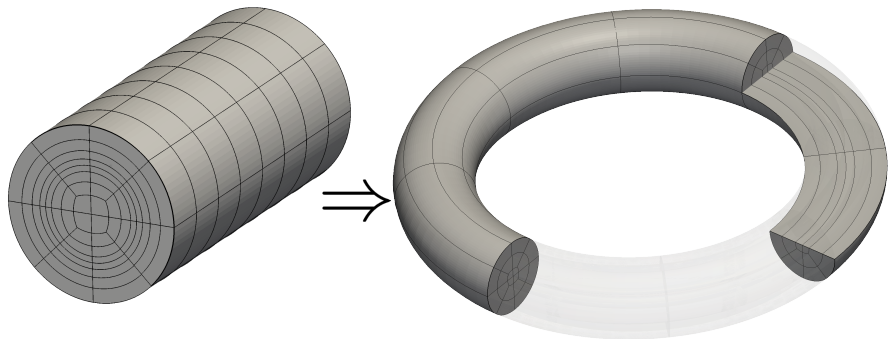
N = 5 & different mesh sizes



N = 3/5/8 on same mesh

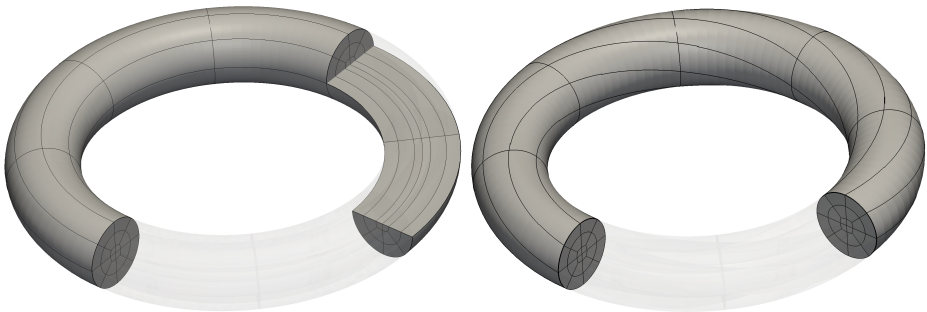
- ▶ Strong scaling on Cray XE6, HLRS Stuttgart
- ▶ Always up to **one element per core**
- ▶ Number of cores is doubled in each step
- ▶ Speedup > 100% owing to cache effects (low memory consumption)
- ⇒ Ideal strong scaling for ≈ 1000 DOF per core, corresponding to **one N8-elem., four N5-elem. or eight N3-elem. per core**

High order meshes



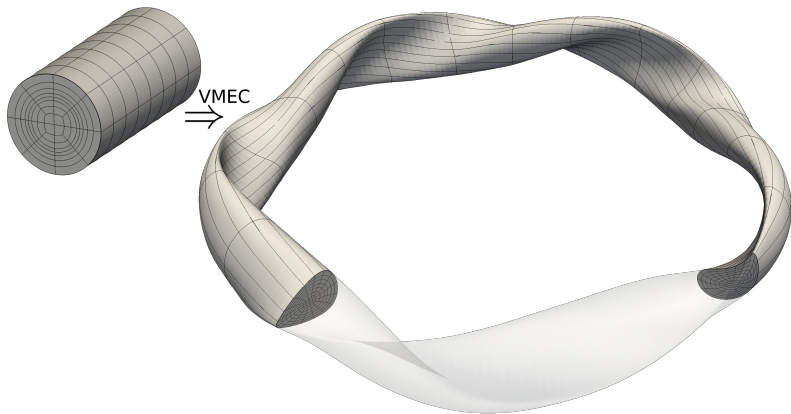
- ▶ Block-structured meshes of cylinder (avoid singularity)
- ▶ High order polynomial element mappings
- ▶ Cylindrical mesh \Rightarrow mapped to torus

High order meshes



- ▶ Mapping approach allows for field alignment in toroidal direction

High order meshes



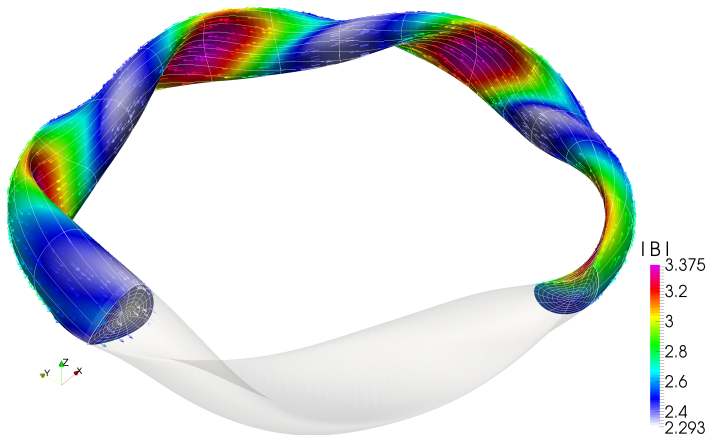
- ▶ **Interface to VMEC:**

Allows to map **Tokamak and Stellarator** configurations:

⇒ get mesh **geometry & MHD equilibrium** ¹

¹VMEC input provided by C. Nuehrenberg, Greifswald

High order meshes



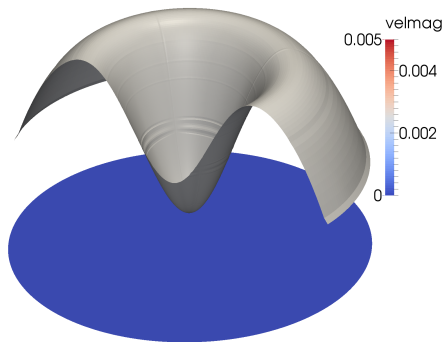
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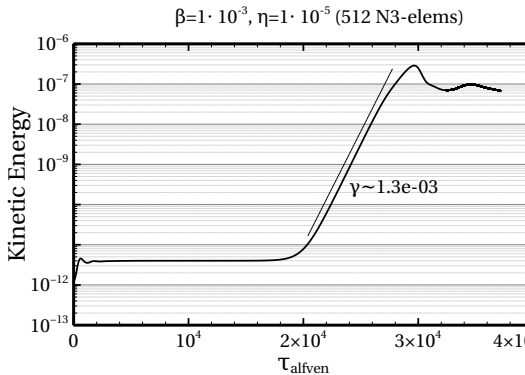
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2D MHD Simulation of a Current Hole Instability



initial current profile

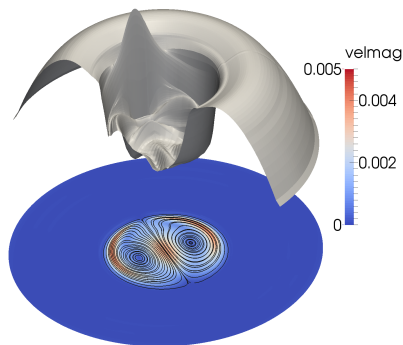


kinetic energy growth

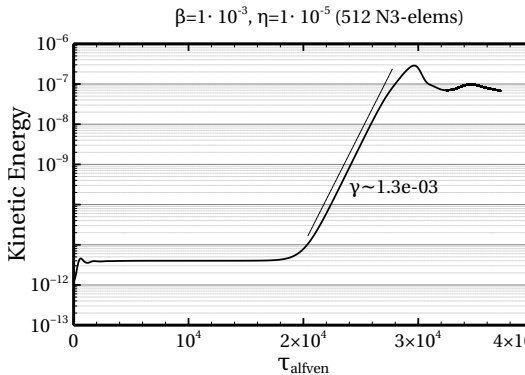
- ▶ Cylindrical domain, 512 N3 elements , setup: Czarny and Huysmans²
 - ▶ MHD equilibrium from radial current profile
- ⇒ Growth rate and solution compares well with reference

²O. Czarny, G. Huysmans, *Bezier surfaces and FE for MHD simulations*, JCP 226, 2008

2D MHD Simulation of a Current Hole Instability



current profile at peak kin. energy

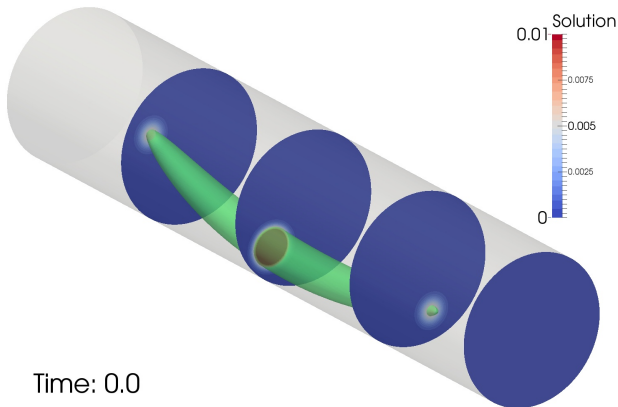


kinetic energy growth

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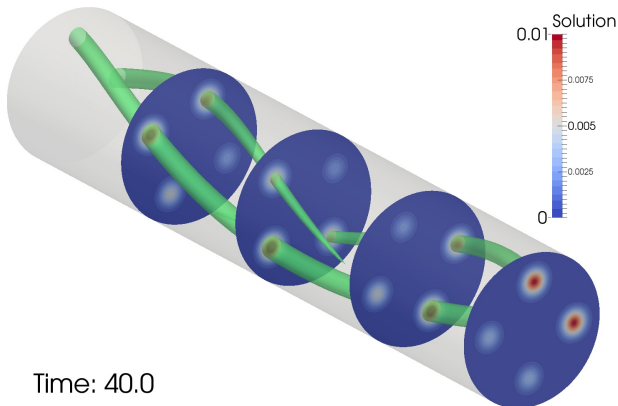
²O. Czarny, G. Huysmans, *Bezier surfaces and FE for MHD simulations*, JCP 226, 2008

Anisotropic diffusion in z-pinch field



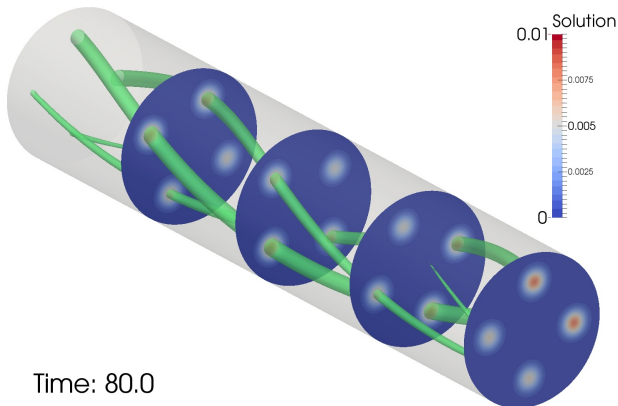
- ▶ Diffusion of a blob in Z-pinch magnetic field
 - ▶ Parallel diff. $\chi_{\parallel} = 1$, perpendicular diff. $\chi_{\perp} = 0$
 - ▶ Periodic cylindrical domain, 1800 N5 elements
- ⇒ Field aligned & same accuracy: factor 8 fewer elements!

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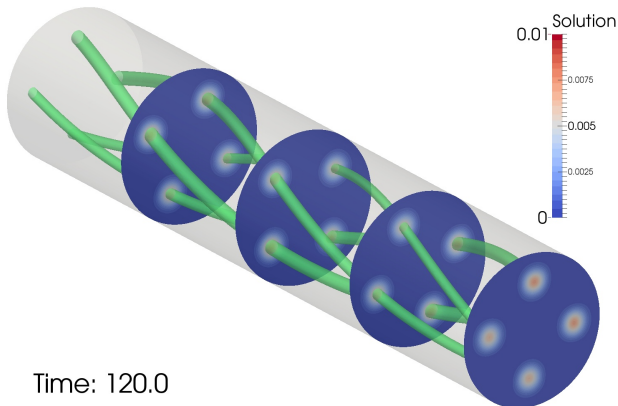
Anisotropic diffusion in z-pinch field



Time: 80.0

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Anisotropic diffusion in z-pinch field



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Outline

Tokamak and stellarator physics

Turbulence and transport: kinetic

Large scale instabilities: MHD

Plasma wave interaction in tokamaks: Maxwell

HPC in the european Fusion community

MHD simulations

Finite Elements: the Jorek Code

Efficient DG code for MHD

Gyrokinetic and kinetic models

Derivation of gyrokinetic model

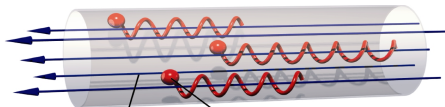
From the continuous to the discrete action: FEM-PIC

Field aligned semi-Lagrangian method

Efficient 6D Vlasov solvers

Numerical issues with 6D Vlasov-Maxwell

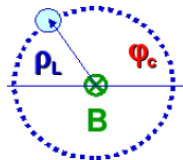
- ▶ **Posed in 6D phase space!** Dimension reduction if possible would help.
- ▶ Large magnetic field imposes **very small time step** to resolve the rotation of particles along field lines.



- ▶ Physics of interest is low frequency. Remove light waves: **Darwin instead of Maxwell**.
- ▶ Debye length small compared to ion Larmor radius. **Quasi-neutrality** assumption $n_e = n_i$ needs to be imposed instead of Poisson equation for electric field.

Towards a reduced model

- ▶ **Scale separation:** fast motion around magnetic field lines can be averaged out.
- ▶ Idea: separate motion of the guiding centre from rotation by a change of coordinates.
- ▶ For constant magnetic field can be done by change of coordinates: $\mathbf{X} = \mathbf{x} - \rho_L$ guiding centre + kind of cylindrical coordinates in \mathbf{v} : v_{\parallel} , $\mu = \frac{1}{2}mv_{\perp}^2/\omega_c$, θ .
- ▶ Mixes position and velocity variables.
- ▶ Perturbative model for slowly varying magnetic field.
- ▶ Several small parameters
 - ▶ **gyroperiod, Debye length**
 - ▶ Magnetic field in tokamak varies slowly: $\epsilon_B = |\nabla B/B|$
 - ▶ Time dependent fluctuating fields are small.



Geometric asymptotic reduction

- ▶ Long time magnetic confinement of charged particles depends on existence of **first adiabatic invariant** (Northrop 1963):
$$\mu = \frac{1}{2}mv_{\perp}^2/\omega_c.$$
- ▶ Geometric reduction based on making this adiabatic invariant an exact invariant.
- ▶ Two steps procedure:
 - ▶ Start from Vlasov-Maxwell **particle Lagrangian** and reduce it using Lie transforms such that it is independent of gyromotion up to second order
 - ▶ Plug particle Lagrangian into Vlasov-Maxwell **field theoretic action** and perform further reduction.
- ▶ End product is **gyrokinetic field theory** embodied in Lagrangian. Symmetries of Lagrangian yield **exact conservation laws** thanks to Noether Theorem.

Historical notes

- ▶ **Perturbative analysis of Vlasov:**
 - ▶ linear: Rutherford & Frieman 68, Taylor & Hastie 68, Catto 78
 - ▶ non linear: Frieman & Chen 82.
- ▶ **Hamiltonian methods:**
 - ▶ electrostatic: Littlejohn 82, 83, Dubin 83
 - ▶ Electromagnetic: Brizard, Lee, Hahm 88, Hahm 88
- ▶ **Gyrokinetic field theory:**
 - ▶ Lagrangian setting: Sugama 2000, Scott & Smirnov 2010
 - ▶ Eulerian setting: Brizard 2000
- ▶ **Review:**
 - ▶ Brizard & Hahm 2007
 - ▶ Krommes 2012, provides a non technical review of the topic.

Motion of a particle in an electromagnetic field

- ▶ Consider given electromagnetic field defined by scalar potential ϕ and vector potential \mathbf{A} such that

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla \phi, \quad \mathbf{B} = \nabla \times \mathbf{A}.$$

- ▶ The **non relativistic equations of motion** of a particle in this electromagnetic field is obtained from Lagrangian (here phase space Lagrangian $\mathbf{p} \cdot \dot{\mathbf{q}} - H$ in non canonical variables for later use)

$$L_s(\mathbf{x}, \mathbf{v}, \dot{\mathbf{x}}, t) = (m_s \mathbf{v} + e_s \mathbf{A}) \cdot \dot{\mathbf{x}}^2 - \left(\frac{1}{2} m_s v^2 + e_s \phi \right).$$

where $\mathbf{p} = m_s \mathbf{v} + e_s \mathbf{A}(t, \mathbf{x})$, $H = m_s v^2/2 + e_s \phi(t, \mathbf{x})$ are canonical momentum and hamiltonian.

Abstract geometric context

- ▶ Lagrangian becomes **Poincaré-Cartan 1-form**

$$\gamma = \mathbf{p} \cdot d\mathbf{x} - H dt$$

with $\mathbf{p} = m_s \mathbf{v} + e_s \mathbf{A}(t, \mathbf{x})$, $H = m_s v^2/2 + e_s \phi(t, \mathbf{x})$.

- ▶ $\omega = d\gamma$ is the Lagrange 2-form, which is non degenerate and so a **symplectic form**. Its components define the the Lagrange tensor Ω .
- ▶ Then $J = \Omega^{-1}$ is the Poisson tensor which defines the Poisson bracket

$$\{F, G\} = \nabla F^T J \nabla G$$

- ▶ The equations of motion can then be expressed from the Poisson matrix and the hamiltonian

$$\frac{d\mathbf{Z}}{dt} = J \nabla H.$$

- ▶ **Lagrangian contains all necessary information** and this structure is preserved by change of coordintates.

Derivation of gyrokinetic particle Lagrangian

- ▶ Gyrokinetic particle Lagrangian obtained from Vlasov-Maxwell particle Lagrangian by performing a change of variables, such that **lowest order terms independent of gyrophase**.
- ▶ This is obtained systematically order by order by the **Lie transform method** (Dragt & Finn 1976, Cary 1981) on the Lagrangian

$$L_s(\mathbf{x}, \mathbf{v}, \dot{\mathbf{x}}, t) = (m_s \mathbf{v} + e_s \mathbf{A}) \cdot \dot{\mathbf{x}}^2 - \left(\frac{1}{2} m_s |\mathbf{v}|^2 + e_s \phi \right).$$

- ▶ Not a unique solution.
 1. v_{\parallel} formulation. Transform Lagrangian as is keeping fluctuation \mathbf{A} in symplectic form.
 2. p_{\parallel} formulation, $p_{\parallel} = v_{\parallel} + (e/m)A_{\parallel}$. Fluctuating A_{\parallel} in hamiltonian.
 3. u_{\parallel} formulation. Split fluctuating A_{\parallel} into two parts. One of them goes into Hamiltonian. **Includes others as special case.**
- ▶ Gyrokinetic codes choose between v_{\parallel} (symplectic) and p_{\parallel} (hamiltonian) formulation.
- ▶ Both involve **severe numerical drawbacks**.

The mixed gyrokinetic particle Lagrangian

- ▶ Split $A_{\parallel} = A_{\parallel}^s + A_{\parallel}^h$. Define $u_{\parallel} = v_{\parallel} + (e/m)A_{\parallel}^h$
- ▶ The gyrokinetic Lagrangian for a single particle always in the form

$$L = \mathbf{A}^* \cdot \dot{\mathbf{X}} + \mu \dot{\theta} - H$$

with $\mathbf{A}^* = \mathbf{A}_0 + \left((m_s/e_s)u_{\parallel} + \langle A_{\parallel}^s \rangle \right) \mathbf{b}$, $\mathbf{b} = \mathbf{B}/B$,

$$H = H_0 + H_1 + H_2, \quad H_0 = \frac{1}{2} m_s u_{\parallel}^2 + \mu B, \quad H_1 = \langle \phi - u_{\parallel} A_{\parallel}^h \rangle$$

where

$$\langle \psi \rangle(\mathbf{x}, \mu) \stackrel{\text{def}}{=} \frac{1}{2\pi} \oint \psi(\mathbf{x} + \rho) d\alpha.$$

- ▶ Perpendicular component of fluctuating vector potential \mathbf{A} neglected.

The Vlasov equation

- ▶ Consider a population of particles evolving with

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}, \quad \frac{d\mathbf{V}}{dt} = \mathbf{F} = \frac{e}{m}(\mathbf{E} + \mathbf{V} \times \mathbf{B}).$$

- ▶ Their distribution function f , or more precisely probability density in phase space (up to normalisation), satisfies the Vlasov equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f = 0.$$

- ▶ Given an initial distribution f_0 , the distribution at time t is equivalently characterised by the solution of the Vlasov equation or the particle positions $f(t, \mathbf{z}) = f_0(X(0; \mathbf{z}, t), V(0; \mathbf{z}, t))$, where we denote by $\mathbf{z} = (\mathbf{x}, \mathbf{v})$.

Action principle for the Vlasov-Maxwell equations

- ▶ Field theory is action principle from which Vlasov-Maxwell equations are derived.
- ▶ Action proposed by Low (1958) with a Lagrangian formulation for Vlasov, *i.e.* based on characteristics.
- ▶ Based on particle Lagrangian for species s , L_s .
- ▶ Such an action, splitting between particle and field Lagrangian, using standard non canonical coordinates, reads:

$$\mathcal{S} = \sum_s \int f_s(\mathbf{z}_0, t_0) L_s(\mathbf{X}(\mathbf{z}_0, t_0; t), \dot{\mathbf{X}}(\mathbf{z}_0, t_0; t), t) d\mathbf{z}_0 dt \\ + \frac{\epsilon_0}{2} \int |\nabla\phi + \frac{\partial \mathbf{A}}{\partial t}|^2 d\mathbf{x} dt - \frac{1}{2\mu_0} \int |\nabla \times \mathbf{A}|^2 d\mathbf{x} dt.$$

Particle distribution functions f_s taken at initial time.

The electromagnetic gyrokinetic field theory

- ▶ Gyrokinetics is a **low frequency approximation**.
Darwin approximation: $\partial_t \mathbf{A}$ removed from Lagrangian.
- ▶ **Quasi-neutrality approximation**: $|\nabla\phi|^2$ removed:

$$\mathcal{S} = \sum_s \int f_s(\mathbf{z}_0, t_0) (\mathbf{A}^* \cdot \dot{\mathbf{X}} - H) d\mathbf{z}_0 - \frac{1}{2\mu_0} \int |\nabla \times (A_{\parallel} \mathbf{b})|^2 d\mathbf{x}.$$

- ▶ Additional approximation made to avoid fully implicit formulation:
Second order term in Lagrangian linearised (consistent with ordering) by replacing full f by background f_M

$$\mathcal{S} = \sum_s \int f_s(\mathbf{z}_0, t_0) (\mathbf{A}^* \cdot \dot{\mathbf{X}} - H_0 - H_1) d\mathbf{z}_0 - \sum_s \int f_{M,s}(\mathbf{z}_0) H_2 d\mathbf{z}_0 - \frac{1}{2\mu_0} \int |\nabla \times (A_{\parallel} \mathbf{b})|^2 d\mathbf{x}.$$

Derivation of the gyrokinetic equations from the action principle

We denote by $\mathbf{B}^* = \nabla \times \mathbf{A}^*$ and $B_{\parallel}^* = \mathbf{B}^* \cdot \mathbf{b}$.

- ▶ Setting $\frac{\delta \mathcal{S}}{\delta Z_i} = 0$, $i = 1, 2, 3, 4$ yields:

$$\mathbf{B}^* \times \dot{\mathbf{R}} = -\frac{m}{q} \dot{P}_{\parallel} \mathbf{b} - \frac{1}{q} \nabla(H_0 + H_1), \quad \mathbf{b} \cdot \dot{\mathbf{R}} = \frac{1}{m} \frac{\partial(H_0 + H_1)}{\partial p_{\parallel}}.$$

- ▶ Solving for $\dot{\mathbf{R}}$ and \dot{P}_{\parallel} we get the **equations of motion of the gyrocenters**:

$$B_{\parallel}^* \dot{\mathbf{R}} = \frac{1}{m} \frac{\partial(H_0 + H_1)}{\partial p_{\parallel}} \mathbf{B}^* - \frac{1}{q} \nabla(H_0 + H_1) \times \mathbf{b}, \quad B_{\parallel}^* \dot{P}_{\parallel} = -\frac{1}{m} \nabla(H_0 + H_1) \cdot \mathbf{B}^*.$$

- ▶ These are the **characteristics of the gyrokinetic Vlasov equation**

$$\frac{\partial f}{\partial t} + \dot{\mathbf{R}} \cdot \nabla f + \dot{P}_{\parallel} \frac{\partial f}{\partial p_{\parallel}} = 0.$$

Gyrokinetic Ampere and Poisson equations

- ▶ The gyrokinetic Poisson (or rather quasi-neutrality) equation is obtained by variations with respect to ϕ

$$\int \frac{e_i^2 \rho_i^2 n_{s,0}}{k_B T_i} \nabla_{\perp} \phi \cdot \nabla \tilde{\phi} \, d\mathbf{x} = \int qn \langle \tilde{\phi} \rangle \, d\mathbf{x}, \quad \forall \tilde{\phi}$$

- ▶ The gyrokinetic Ampère equation is obtained by variations with respect to A_{\parallel} :

$$\begin{aligned} \int \nabla_{\perp} A_{\parallel} \cdot \nabla_{\perp} \tilde{A}_{\parallel}^h \, d\mathbf{x} + \sum_s \int \frac{\mu_0 q_s^2 n_s}{m_s} \langle A_{\parallel}^h \rangle \langle \tilde{A}_{\parallel}^h \rangle \, d\mathbf{x} \\ = \mu_0 \int j_{\parallel} \langle \tilde{A}_{\parallel}^h \rangle \, d\mathbf{x}, \quad \forall \tilde{A}_{\parallel}^h \end{aligned}$$

- ▶ where $A_{\parallel} = A_{\parallel}^s + A_{\parallel}^h$ and A_{\parallel}^s is related to ϕ by the constraint

$$\frac{\partial A_{\parallel}^s}{\partial t} + \nabla \phi \cdot \mathbf{b} = 0.$$

Conserved quantities

- ▶ Symmetries of Lagrangian yield invariants using Noether's theorem
- ▶ Time translation: **Conservation of energy:**

$$\mathcal{E}(t) = \sum_s \int dW_0 dV_0 f_{s,0}(\mathbf{z}_0) H_s - \int dV \frac{e_i^2 \rho_i^2 n_{s,0}}{k_B T_i} |\nabla \phi|^2 + \frac{1}{2\mu_0} \int dV |\nabla_{\perp} A_{\parallel}|^2.$$

- ▶ Axisymmetry of background vector potential:
Conservation of total canonical angular momentum:

$$\mathcal{P}_{\varphi} = \sum_s e_s \int dW_0 dV_0 f_{s,0}(\mathbf{z}_0) \mathbf{A}_{s,\varphi}^*$$

Discretisation of the action

- ▶ Our action principles rely on a **Lagrangian (as opposed to Eulerian) formulation of the Vlasov equation**: the functionals on which our action depends are the characteristics of the Vlasov equations \mathbf{X} and \mathbf{V} in addition to the scalar and vector potentials ϕ and \mathbf{A} .
- ▶ A natural discretisation relies on:
 - ▶ A Monte-Carlo discretisation of the phase space at the initial time: select randomly some initial positions of the particles.
 - ▶ Approximate the continuous function spaces for ϕ and \mathbf{A} by discrete subspaces.
 - ▶ Yields a discrete action where a finite (large) number of scalars are varied: the particle phase space positions and coefficients in Finite Element basis.
- ▶ When performing the variations, we get the classical **Particle In Cell Finite Element Method (PIC-FEM)**.

FEEC needed for Maxwell's equations

- ▶ In order to preserve the continuous structure at the discrete level, the different unknowns ϕ , \mathbf{A} , \mathbf{E} and \mathbf{B} need to be chosen in compatible Finite Element spaces.
- ▶ This is provided by Finite Element Exterior Calculus (FEEC) introduced by Arnold, Falk and Winther.
- ▶ Continuous and discrete complexes are the following

$$\begin{array}{ccccccc}
 & \mathbf{grad} & & \mathbf{curl} & & \mathbf{div} & \\
 H^1(\Omega) & \longrightarrow & H(\mathbf{curl}, \Omega) & \longrightarrow & H(\mathbf{div}, \Omega) & \longrightarrow & L^2(\Omega) \\
 \downarrow \Pi_0 & & \downarrow \Pi_1 & & \downarrow \Pi_2 & & \downarrow \Pi_3 \\
 V_0 & \longrightarrow & V_1 & \longrightarrow & V_2 & \longrightarrow & V_3
 \end{array}$$

- ▶ Faraday and $\mathbf{div} \mathbf{B} = 0$ verified strongly as

$${}^1\mathbf{E} = -\nabla^0\phi - \frac{\partial {}^1\mathbf{A}}{\partial t}, \quad {}^2\mathbf{B} = \nabla \times {}^1\mathbf{A}.$$

- ▶ Ampere and Gauss' law obtained from variations of FE coefficients.

PIC Finite Element approximation of the Action

- ▶ Compatible FE discretisation:

$$\phi_h \in V_0, \quad \mathbf{A}_h, \mathbf{E}_h \in V_1, \quad \mathbf{B}_h \in V_2.$$

- ▶ Particle discretisation of $f \approx \sum_k w_k \delta(x - x_k(t)) \delta(v - v_k(t))$
- ▶ Vlasov-Maxwell action becomes:

$$\begin{aligned} \mathcal{S}_{N,h} = & \sum_{k=1}^N w_k L_s(\mathbf{Z}(\mathbf{z}_{k,0}, t_0; t), \dot{\mathbf{Z}}(\mathbf{z}_{k,0}, t_0; t), t) - \frac{1}{2} \int \left| \sum_{i=1}^{N_g} a_i(t) \nabla \times \Lambda_i^1(\mathbf{x}) \right|^2 d\mathbf{x} \\ & + \frac{1}{2} \int \left| \sum_{i=1}^{N_g} \phi_i(t) \nabla \Lambda_i^0(\mathbf{x}) + \sum_{i=1}^{N_g} \frac{da_i(t)}{dt} \Lambda_i^1(\mathbf{x}) \right|^2 d\mathbf{x}. \end{aligned}$$

- ▶ $\mathbf{Z}(\mathbf{z}_{k,0}, t_0; t)$ will be traditionally denoted by $\mathbf{z}_k(t)$ is the phase space position at time t of the particle that was at $\mathbf{z}_{k,0}$ at time t_0 .

PIC-FE discretisation of the action

- ▶ We know have a discrete action depending on particle positions and Finite Element degrees of freedom, which define the generalised coordinates

$$\mathcal{S}_{N,h}[\mathbf{x}_1, \dots, \mathbf{x}_N, \dot{\mathbf{x}}_1, \dots, \dot{\mathbf{x}}_N, \mathbf{v}_1, \dots, \mathbf{v}_N, \phi_1, \dots, \phi_{N_g}, a_1, \dots, a_{N_g}]$$

- ▶ The discrete electric and magnetic fields are defined exactly as in the continuous case from the discrete potentials thanks to the compatible Finite Element spaces

$$\mathbf{E}_h = \sum_i e_i \Lambda_i^1(\mathbf{x}) = -\nabla \phi_h - \frac{\partial \mathbf{A}_h}{\partial t}, \quad \mathbf{B}_h = \sum b_i \Lambda_i^2(\mathbf{x}) = \nabla \times \mathbf{A}_h.$$

- ▶ It immediately follows like in the continuous case the discrete Faraday equation

$$\frac{\partial \mathbf{B}_h}{\partial t} + \nabla \times \mathbf{E}_h = 0.$$

Time advance via Hamiltonian splitting

- ▶ Following the prescription of Crouseilles-Einkemmer-Faou a Hamiltonian splitting can be performed, treating the three terms of the Hamiltonian separately

$$H = \frac{1}{2} \mathbf{v} M_p \mathbf{v} + \frac{1}{2} \mathbf{e} M_1 \mathbf{e} + \frac{1}{2} \mathbf{b} M_2 \mathbf{b} = H_p + H_e + H_b.$$

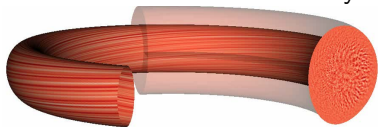
- ▶ Split and solve successively ($\Omega(u)$ Poisson matrix)

$$\frac{du}{dt} = \Omega(u) \nabla H_i, \quad i = p, e, b$$

- ▶ Lie-Trotter splitting (first order), Strang splitting (second order) or even higher order.
- ▶ Exact solution possible for H_e and H_b .
- ▶ For H_p split further between the three components. Other possibility: use variational integrator

Comments and related work

- ▶ Variational FE-PIC codes along with control variates for noise reduction at the base of success of PIC simulations of Tokamak turbulence with ORB5 family of codes.



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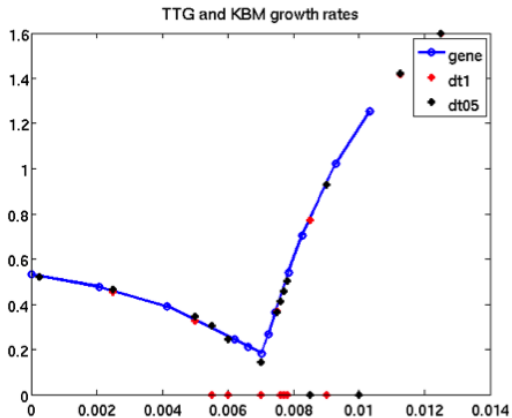
(Picture: A. Bottino)

- ▶ A lot of recent effort towards variational or Hamiltonian discretisation of Vlasov (or related)
 - ▶ First ref: Lewis, Energy conserving numerical approximations of Vlasov plasmas, JCP 1970
 - ▶ Shadwick, Stamm, Estatiev, Variational formulation of macro-particle plasma simulation algorithms (Phys Plasmas 2014)
 - ▶ Squire, Qin, Tang, Geometric integration of the Vlasov-Maxwell system with a variational particle-in-cell scheme, (Phys Plasmas 2012)

- ▶ European project VeriGyro:
 - ▶ Most popular tools for plasma turbulence investigation
 - ▶ Extended development over last 10 years
 - ▶ Variety of implemented GK models
- ▶ Building up hierarchy of Gyrokinetic models implemented into the codes:
 - ▶ Systematic derivation from the Variational GK framework
 - ▶ Verification of approximations consistency
 - ▶ Identification of regimes of applicability
- ▶ Intercode Benchmark: implicit numerical schemes verification
 - ▶ Hierarchy of numerical test cases: from adiabatic electrons towards linear electromagnetic simulation.
 - ▶ Participating codes: GENE/GKW (Eulerian); ORB5/EUTERPE (PIC); GYSELA (Semi - Lagrangian)

Linear electromagnetic benchmark

- ▶ Second order Gyrokinetic theory for Particle-In-Cell code ORB5
- ▶ Intercode linear electromagnetic Benchmark (ORB5 & GENE)
- ▶ Identification of instabilities transitions: from ITG (low frequencies) to KBM (high frequencies)

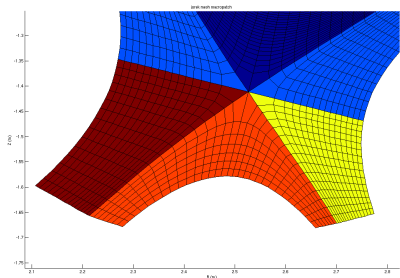


Ultimate Goals

- ▶ Gyrokinetics: non-linear, electromagnetic, with multiple species
- ▶ Complex 3D geometries (Tokamaks and Stellarators)
- ▶ Global simulations (including magnetic axis and X point)

Opposing Requirements

- ▶ **Efficiency**: minimize number of degrees of freedom
- ▶ **Geometry**: flexible and robust 3D meshing, e.g. mapped multiblock grids (see figure)



Observation

- ▶ Linear instability modes have large parallel wavelengths ($\lambda_{\parallel} \gg r_{Li}$)
- ▶ Turbulence structures also have small parallel gradients ($\nabla_{\parallel} \ll \nabla_{\perp}$)

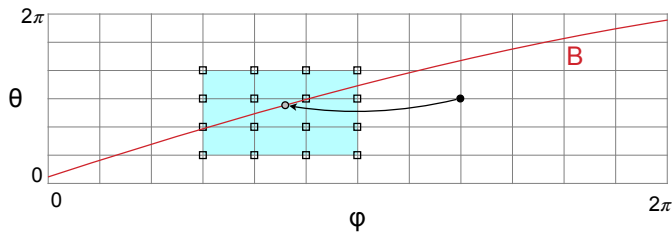
Magnetic flux coordinates

- ▶ Allow for great reduction of grid points along one direction
- ▶ Shortcomings: singularities (magnetic axis, X-point), complex meshing, inhomogenous grid spacing

Field-aligned approach

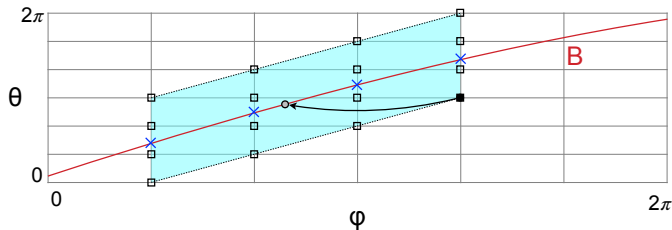
- ▶ Allows reduction of grid points along toroidal direction φ
- ▶ Great mesh flexibility, uses interpolation on poloidal plane

Gyrokinetics: field-aligned semi-Lagrangian schemes



Standard Interpolation

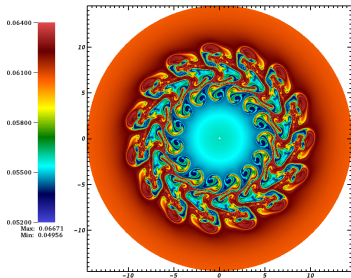
- ▶ centered rectangular stencil
- ▶ requires fine mesh in φ



Field-Aligned Interpolation

- ▶ stencil adapts to magnetic field line
- ▶ allows for coarser mesh in φ

Gyrokinetics: field-aligned semi-Lagrangian schemes



Progress in SeLaLib

- ▶ ITG instability in screw-pinch geometry
- ▶ Uniform mesh in polar coordinates
- ▶ Verification: growth rates match analytics
- ▶ Figure: distribution function at $\varphi = 0$, $v_{\parallel} = 0$

	Geometry	Equations
Current State	theta-pinch screw-pinch cylindrical Tokamak (in Gysela)	gyrokinetic ($\mu = 0$) ions adiabatic electrons electrostatic limit
Next Steps	bumpy-pinch (straight stellar.) Tokamak (Asdex-U, ITER) Stellarator (Wendelstein 7-X)	fully gyrokinetic ions gyrokinetic ($\mu = 0$) electrons electromagnetic

Vlasov equation in 6D

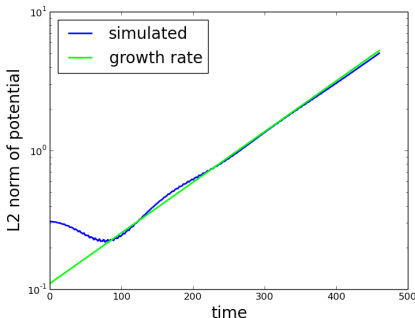
Goal:

- ▶ Develop efficient semi-Lagrangian solver of Vlasov equation in 6D
- ▶ Study physical problems to verify/improve gyrokinetics

First test case: Simulation of ITG in slab with periodic boundary conditions

Verification: Comparison to dispersion relation

- ▶ frequency: dispersion
 $\omega_r \approx -0.01854$,
 simulated $\omega_r \approx -0.0185$
- ▶ growth rate: see figure



Two approaches:

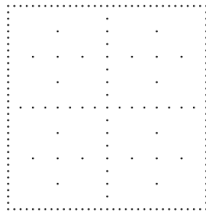
- ▶ Remap: Work with two domain partitions, one keeping the spatial coordinates local and one keeping the velocity coordinates local \rightsquigarrow transpose of data in all-to-all communication.
- ▶ Domain decomposition (DD): Work with one domain partitioning which consists of 6D subblocks of the total data \rightsquigarrow neighbor-neighbor communication.

Results:

- ▶ Data exchange dominates.
- ▶ Lagrange interpolation better suited for DD than splines.
- ▶ DD allows for optimizations by exchange of data in 32-bit and compression.

6D Vlasov solver on sparse grids

Idea of sparse grids: Down-sampling of full grid to reduce the curse of dimensionality in an optimal way for a given class of functions.



from: Garcke, Sparse grid tutorial

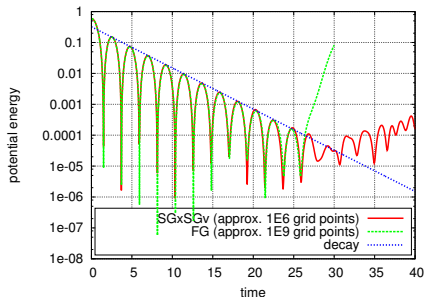
Key features of the solver:

- ▶ Representation of the distribution function on tensor product of sparse grids in x and v .
- ▶ Propagation with semi-Lagrangian method: Combine sparse-grid interpolation with 1D spline interpolation.
- ▶ Multiplicative δf -method: Only a (multiplicative) deviation from an equilibrium state is represented on the sparse grid.

6D Vlasov solver on sparse grids

Results:

- ▶ Good compression can be achieved if close to equilibrium
- ▶ Numerical instabilities can occur if problem is severely underresolved



Next steps:

- ▶ Improve parallelization strategy for 6D solver.
- ▶ Consider configurations with magnetic fields with sparse grid or low-parametric tensor solver.

Tensor train representation

- ▶ Very efficient solver with optimal complexity ($O(N)$ or $O(N \log_2 N)$) has been developed for 6D Vlasov-Poisson equations.
- ▶ However 6D grid is huge: e.g. $N = 64^6 \approx 70 \times 10^9$.
- ▶ Idea: Use **low-rank tensor representation**

$$Q(x_1, \dots, x_d) = \sum_{\alpha_1, \dots, \alpha_{d-1}} Q_1(x_1, \alpha_1) Q_2(\alpha_1, x_2, \alpha_2) \dots Q_d(\alpha_{d-1}, x_d)$$

to represent the data more efficiently.

- ▶ Semi-Lagrangian method developed within the **Tensor Train** framework.
- ▶ Result: Data compression but more complex algorithms (QR and SVD of the kernels to recompress data).

Prototype MATLAB implementation

- ▶ Nonlinear Landau damping problem.
Computing time (wall clock time) and memory of a tensor representation (TT) compared to the solution on the full grid (FG) for 1146 iterations.

dim	method	# doubles for f	fraction	wall time	fraction
2D	FG	4096		$1.5 \cdot 10^1$	
2D	TT	2720	0.66	$6.8 \cdot 10^0$	0.45
4D	FG	$1.7 \cdot 10^7$		$6.2 \cdot 10^4$	
4D	TT	$5.5 \cdot 10^4$	$3.3 \cdot 10^{-3}$	$6.0 \cdot 10^2$	$9.7 \cdot 10^{-3}$
6D	TT	$3.1 \cdot 10^6$	$4.5 \cdot 10^{-5}$	$2.7 \cdot 10^4$	

Next steps

- ▶ High-performance implementation based on efficient dense linear algebra packages.
- ▶ Solution of Vlasov–Maxwell equations.

Conclusions and perspectives

- ▶ Applied math and HPC a strong need of magnetic fusion research
- ▶ Very complex models. Solid theory and verification strategy required.
- ▶ Gyrokinetic and kinetic simulations posed in 5D or 6D phase space require a lot of resources and scale well with some effort.
- ▶ Verification and development based on modern software engineering concepts needed.