GenFoo: a general Fokker-Planck solver with applications in fusion plasma physics

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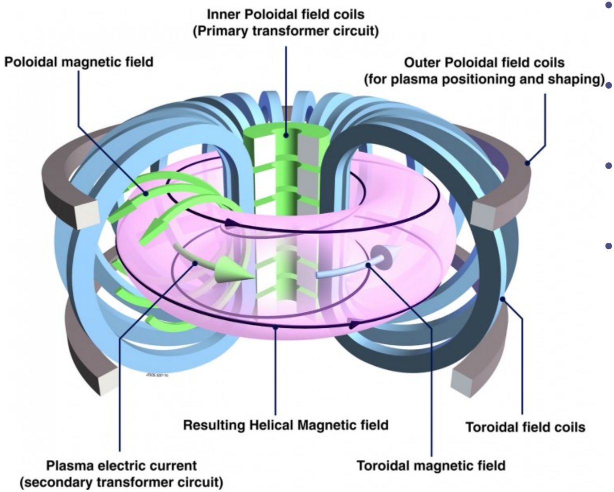
June 6, 2012

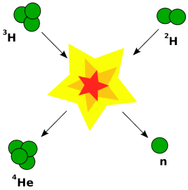
Outline

- Fusion energy
- Integrated Tokamak Modeling and ITER
- Kinetic diffusion: Coulomb collisions
- GenFoo: a general Fokker-Planck solver
- Summary

Magnetic confinement fusion



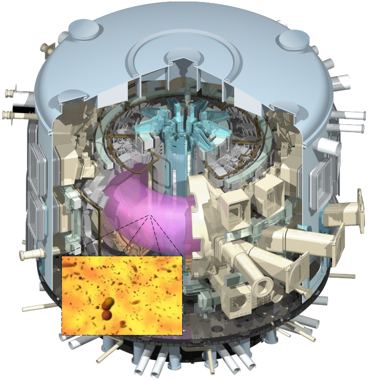
- D+T => He4 + n + 17.59 Mev
- Temperature at around 200 million degrees (K)
- Confined by magnetic fields
- Huge temperature gradients => turbulent plasma



The ITER project

"To demonstrate that it is possible to produce commercial energy from fusion."

- Output power 500 MW, input power 50 MW
- Height: 73 metres
- Weight: 23,000 tons
- Cost: 13 billion euros



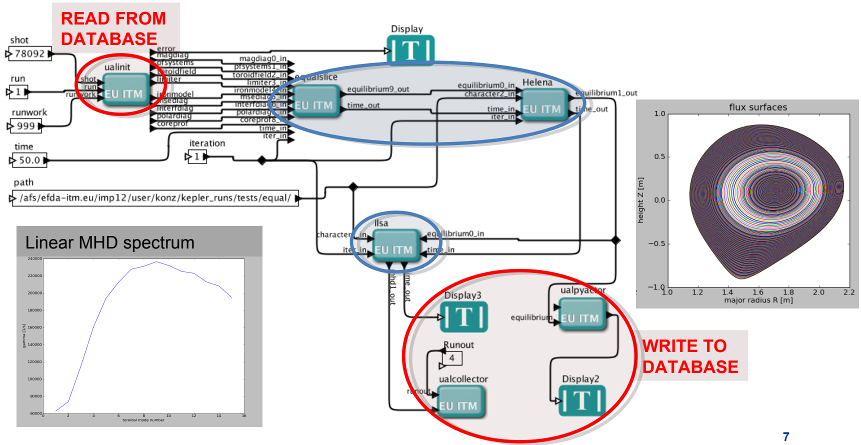
Integrated Tokamak Modeling Task Force in EU

"The main mission of ITM-TF is to build a validated suite of simulation codes for ITER plasmas and to provide a software infrastructure framework for EU integrated modeling activities." from efda-itm.eu

- Aim to offer a full simulation environment.
- Provide a validated set of European modeling tools for ITER exploitation.
- Provide an API for coupled codes written in different languages.

Simple workflow in Kepler

- Kepler: a graph based workflow tool for coupling ITM codes, kepler-project.org



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Spatio-temporal scales in plasma kinetic models

- The physics in a confined heated plasma occur on a broad range of temporal and spatial scales.
- Spatial scales from the electron gyroradius, 10^{-6}m to the size of the confinement device 10^{1}m.
- Temporal scales range from the electron gyroperiod, 10^{-10}s to the plasma pulse length 10^{5}s.
- Requires the [1]largest computational facilities in the world.

[1] Currently the K-computer in Japan (figure), with 10 petaflops per second

The kinetic description of charged particles

$$\frac{\partial}{\partial t} f_a(\mathbf{r}, \mathbf{v}, t) + \mathbf{v} \cdot \frac{\partial f_a}{\partial \mathbf{r}} + \frac{e_a}{m_a}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f_a}{\partial v} = \left(\frac{\partial f_a}{\partial t} \right)_c$$

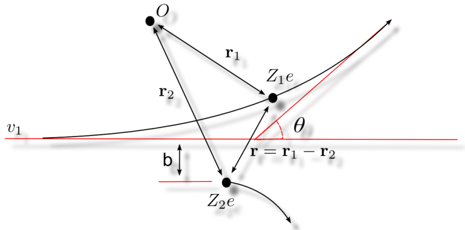
$$\left(\frac{\partial f_a}{\partial t} \right)_c = \sum_b C_{ab}(f_a, f_b)$$

Properties:

- 6D+1 dimensional
- l.h.s. describes evolution of particle distribution on a macroscopic scale while r.h.s. models coulomb collisions on a microscopic scale.

Coulomb collisions

- The Coulomb collision process describes collisions between charged particles:



- Dominated by small angle, long range collision in contrast to large angle, binary collision in neutral gases.

The collision operator

- Decorrelation allow collisions to be modeled as a $3+1$ dimensional nonlinear Fokker-Planck equation:

$$\left(\frac{\partial}{\partial t}f_a\right)_c = -\sum_{i}^{3}\frac{\partial}{\partial v_i}A_i(\mathbf{v},f_a,f_b)f_a + \frac{1}{2}\sum_{i,j}^{3}\frac{\partial}{\partial v_i}B_{i,j}(\mathbf{v},f_a,f_b)\frac{\partial}{\partial v_j}f_a$$

where $A = C_a\nabla\phi(\mathbf{v})$, $\mathbf{B} = C_s\nabla\nabla\Psi(\mathbf{v})$ and

$$\phi(\mathbf{v}) = -\frac{1}{4\pi}\int\frac{f_b(\mathbf{v}')}{|\mathbf{v}-\mathbf{v}'|}d^3(\mathbf{v}')$$

$$\Psi(\mathbf{v}) = -\frac{1}{8\pi}\int|\mathbf{v}-\mathbf{v}'|f_b(\mathbf{v}')d^3(\mathbf{v}')$$

are the so called Rosenbluth potentials.

- It describes the evolution of a probability density on a mesoscopic scale.

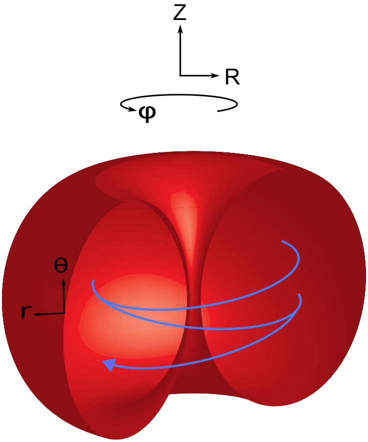
Dimension reduction by symmetries

- Orbit averaging over the periodic action angle variables (the angles in action-angle system); gyro angles α, bounce angle β and toroidal angle ϕ.

$$\frac{\partial f_a}{\partial t} = \nabla_{\mathbf{v}} \cdot (-\langle \mathbf{A} \rangle \cdot f_a + \langle \mathbf{B} \rangle \cdot \nabla_{\mathbf{v}} f_a)$$

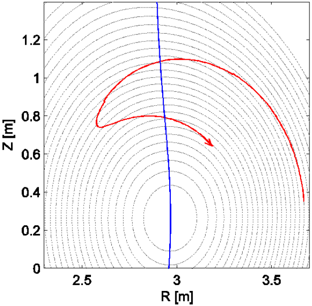
where
$\langle X \rangle = \frac{1}{(2\pi)^3} \int X d\phi d\beta d\alpha$.

- Orbit averaging reduces the 6D problem to a 3D adiabatic invariant space with complex internal boundaries.



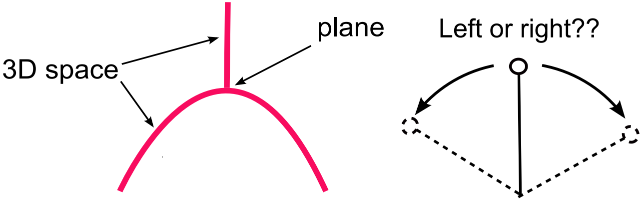
Challenges of the adiabatic invariant model

Drift $\langle \mathbf{A} \rangle$ and diffusion $\langle \mathbf{B} \rangle$ coefficients must be calculated numerically with external codes. They contain line integrals over the particle orbit



$$\langle g \rangle = (2\pi)^{-1} \oint g(R(\beta), Z(\beta)) d\beta$$

- The space contains a bifurcation,

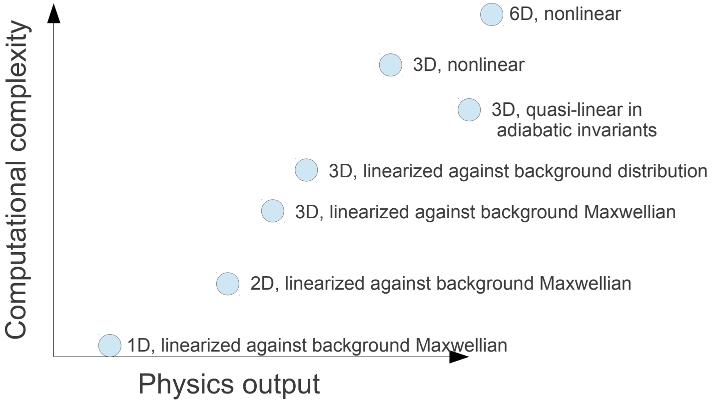


Model reduction

- Homogenize in **r** and assume local isotropy in velocity space => 1D-2D Fokker-Planck models however with singular drift and diffusion coefficients
- Linearize:
  - Assume collisions against a known distribution, $C(f_a, f_b)$ where f_b is known.
  - Rosenbluth potentials have analytical solutions if f_b is a local Maxwellian.

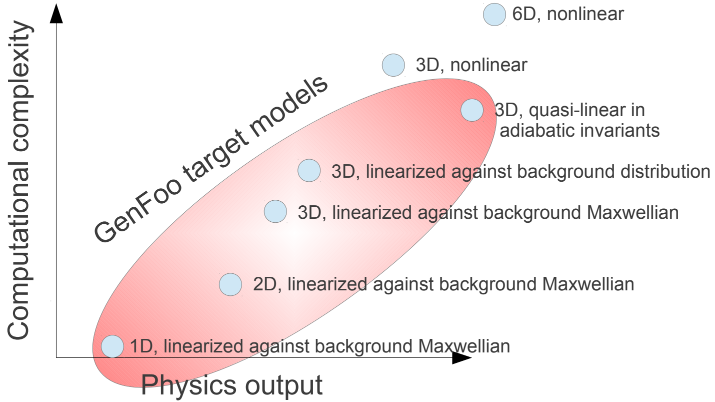
Computational complexity vs physics output

Different Fokker-Planck models



Computational complexity vs physics output

Different Fokker-Planck models



GenFoo, GEneral FOkker-Planck sOlver

- Separate numerics and physics with an API for the operator coefficients.
- Numerics: FEM or (δf) Monte-Carlo.
- Physics: convection + diffusion + source + initial values.
- XML in and XML out design => compatible with XProc, the XML pipeline language, w3.org/TR/xproc.
- Monte Carlo particles are stored in the h5Part (HDF5 4 particles, vis.lbl.gov/Research/H5Part) format.

GenFoo solves ...

- the Fokker-Planck equation in n variables $\mathbf{x} = x_1, \ldots, x_n$,

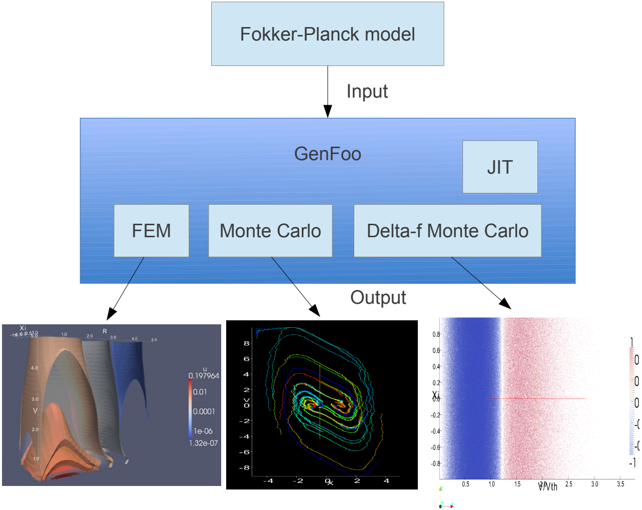
$$\frac{\partial f}{\partial t}(\mathbf{x}, t) = -\sum_i^n \frac{\partial}{\partial x_i} A_i(\mathbf{x}) f(\mathbf{x}, t) + \frac{1}{2} \sum_{i,j}^n \frac{\partial^2}{\partial x_i \partial x_j} B_{ij}(\mathbf{x}) f(\mathbf{x}, t) + H(\mathbf{x})$$

  assuming natural boundary conditions where A_i and B_{ij} are the drift vector and diffusion tensor respectively.
- The *characteristics* are described by an Itô stochastic differential equation (SDE)

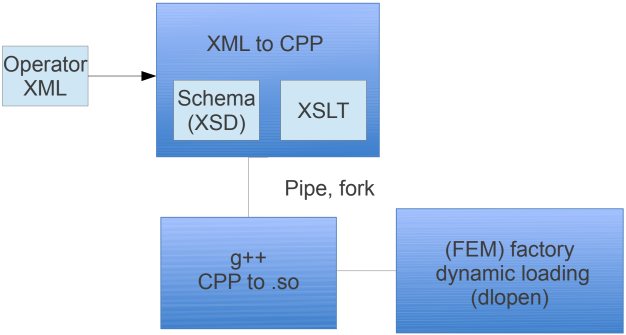
$$dX_i(t) = A_i(X(t))dt + \sum_j^q \sigma_{ij}(X(t))dW_j(t)$$

  where σ_{ij} is defined by $B_{ij} = \sum_k^q \sigma_{ik}\sigma_{kj}$ and dW is a q-dimensional Wiener process with zero mean and dt variance.
- Many realizations of the SDE give a distribution with the same solution as obtained by the FPE.

Internal structure of GenFoo



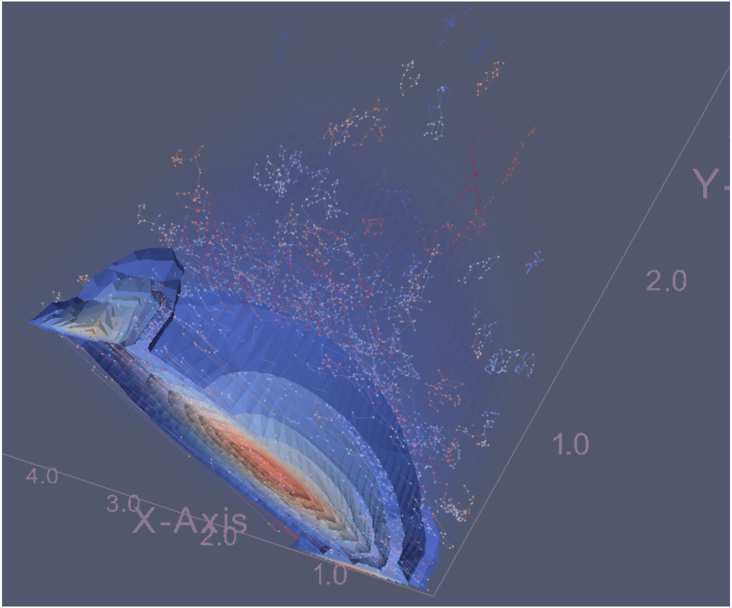
The JIT compiler



Defining an operator: Heston model in finance

```xml
<?xml version="1.0"?>
<Operator>
 <Dimensions> 2 </Dimensions>
   <Drift>
    <component index="0"> <value> (r-d)*x[0] </value> </component>
    <component index="1"><value>kappa*(theta-x[1])</value></component>
   </Drift>
   <Diffusion>
    <component indexColumn="0" indexRow="0" >
      <value> sqrt(x[1])*x[0] </value>
    </component>
    <component indexColumn="1" indexRow="1">
      <value> xi*sqrt(abs(x[1])) </value>
    </component>
   </Diffusion>
   <Source> <value>0.0</value></Source>
   <InitialCondition><value> ...</value></InitialCondition>
</Operator>
```

3D radio-frequency heating



GenFoo blueprints

Implement...

- a common plasma physics class.
- stability schemes e.g. SUPG, standard Galerkin on augmented grid [Brezzi, 2005], suggestions are welcome!
- time-dependent goal-oriented adaptivity.
- output kernels.

Summary

GenFoo target plasma physics models with the properties:

- singular coefficients and local convection dominated regions.
- two dimensional bifurcation plane in three dimensional space.

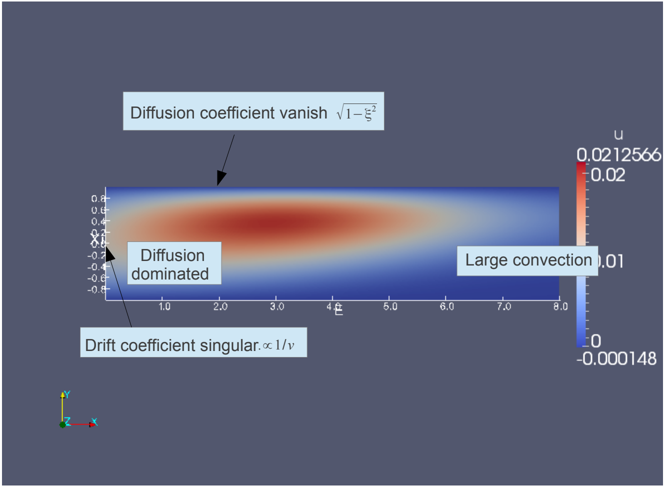
The GenFoo wish list: FEniCS support for ...

- goal-oriented (auto) adaptivity for time-dependent problems.
- 6D models
- perhaps support for ADIOS (the Adaptable IO System, olcf.ornl.gov/center-projects/adios).

Thank you!

Extra slides

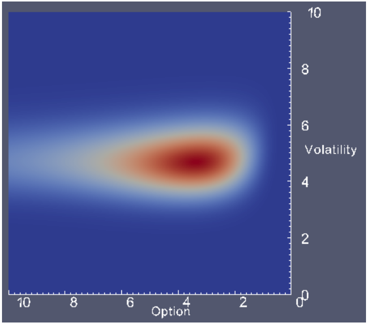
A linearized isotropic Coulomb collision model



Running GenFoo

Cmd: mpirun -np 4 ./GenFoo ../Params/Heston.xml

```
<library>
<filename>../Operators/XML/HestonModel.xml
</filename>
</library>
<factory>
   <select>FEM</select>
   <FEM>
     <gridSize> 100 100</gridSize>
     <solver> gmres </solver>
   </FEM>
...
</factory>
...
```



A XML scheme for output kernels

$$\int K(p_0, \ldots, p_i) f(p_0, \ldots, p_i) dp_k, \ldots, dp_l$$

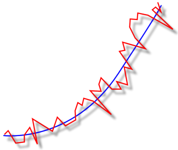
```
<GenFooOutputSpecification ... programmingLanguage="c++">
 <integralMeasure name="distributioninEnergyAndMinorRadius"
type="contraction">
  <geometry>
   <dimensions> 0 2 </dimensions>
   <gridSize> 200 55 </gridSize>
   <minValue> -1 0 </minValue>
   <maxValue> 1 1 </maxValue>
  </geometry>
  <kernelCode>return 1.0; </kernelCode>
 </integralMeasure>
</GenFooOutputSpecification>
```

- A schema exists, parser yet to be implemented

Stochastic differential equations (SDE)

- An ordinary differential equation with an extra noise term:

$$\frac{dV(t)}{dt} = f(V,t) + \text{"random noise"}.$$



- The Itô stochastic differential equation (SDE):

$$dV(t) = A(V(t),t)dt + \sigma(V(t),t)dW(t), \quad t_0 \leq t \leq T$$

where $dW(t)$ is the Wiener process (Brownian motion).

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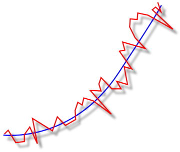

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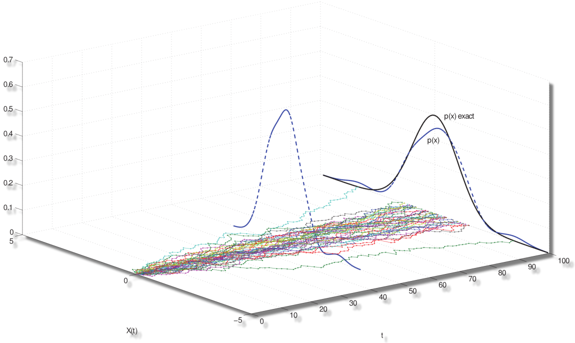
Link between SDEs and the FP equation

- Many realizations of the SDE give a density of particles with the distribution function *P* solved by the Fokker-Planck equation:



$$E[V(T)|V(t_0) = v] = \int g(y)P(y, T; v, t_0)dy.$$