Computational plasma physics – extending legacy codes, computing functionals and other ideas

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Markus Hegland, ANU

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Introduction

Overview

challenges in computational science and engineering

- exascale computing
  - faults
  - synchronisation and communication
  - new approximations
- assimilating data with computational solutions of PDEs
- including extensive computations in control
- uncertainty in models, data and computations
- managing very complex computational codes
- focus on quantities of interest and dual problems
  - inverse problems and optimisation

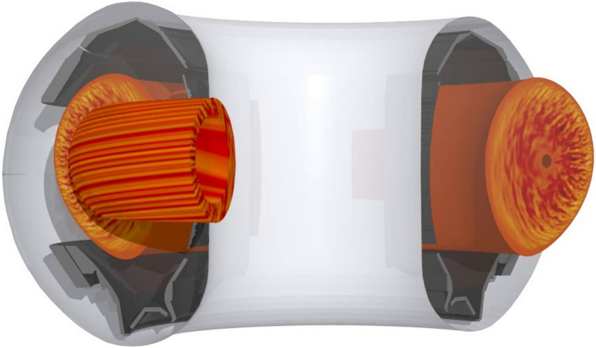
role of mathematics

- enhance understanding of assumptions and observations used in code development
- approximation errors in legacy and new code
- complexity
- properties of models (e.g. PDE existence and uniqueness theorems)
- error propagation
- understanding the nature of collaborations and role of different disciplines
    - people are interdisciplinary

our project

- code base: GENE – development lead by Frank Jenko, IPP Munich
  - highly scalable, tested on various HPCs
  - international user base
  - under constant development
- our aim: extending the capability of GENE without changing the core
  - approach: numerical extrapolation based on multiple simulations with different grid parameters
  - applications: solve larger problems, parameter optimisation, uncertainty quantification
- resources: 4 PhD students, ARC Linkage project with Fujitsu Europe and collaboration with TU Munich through DFG excellence initiative
- so far: fault tolerant sparse grids
- target: mathematics behind GENE computations
- in this talk: explore approximations used

GENE



- open source plasma research code
- state of the art, highly optimised for high performance computers
- our work: utilise sparse grids to improve performance and fault tolerance

Collaborators

This talk is based on past and current collaborative research with Yuancheng Zhou (ANU), Christoph Kowitz (formerly TU Munich), Brendan Harding (UoA), Peter Strazdins (ANU), Peter Vasiliou (ANU), Matthew Hole (ANU), Stuart Hudson (PPL Princeton), Frank Jenko (MPI Garching) and Dirk Pfluger (Uni Stuttgart)

Approximation 1: PDEs approximating ODEs

dynamics of a single particle

- **Newton's equations** for charged particles

$$\frac{d}{dt}\begin{bmatrix} x \\ v \end{bmatrix} = \begin{bmatrix} v \\ \frac{1}{m}F(x,v) \end{bmatrix}$$

  - Lorentz force $F(x,v) = q(E + v \wedge B)$
- **Hamilton's equations**

$$\frac{d}{dt}\begin{bmatrix} x \\ p \end{bmatrix} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \nabla H$$

  - Hamiltonian $H(x,p) = \frac{1}{2m}\|p - \frac{q}{c}A\|^2 + \phi(x)$
  - fields $E = \nabla\phi - \frac{\partial A}{\partial t}$ and $B = \nabla \wedge A$
  - momentum $p = v + \frac{q}{c}A$

Maxwell's equations

$$\frac{\partial E}{\partial t} = c^2 \nabla \wedge B - \frac{j}{\epsilon_0}$$
$$\frac{\partial B}{\partial t} = -\nabla \wedge E$$

and

$$\nabla \cdot E = \frac{\rho}{\epsilon_0}$$
$$\nabla \cdot B = 0$$

solutions

$$E = -\nabla \phi - \frac{\partial A}{\partial t}$$
$$B = \nabla \wedge A$$

where

$$\phi(x, t) = \int \frac{\rho(\xi, t - r/c)}{2\pi\epsilon_0 r} d\xi$$
$$A(x, t) = \int \frac{j(\xi, t - r/c)}{2\pi\epsilon_0 r} d\xi$$

and $r = \|x - \xi\|$

- GENE solves Poisson-Ampere equations

Vlasov equations

- let $X(t)$ and $V(t)$ solve Newton's equations
- let $\mu_0(x, v)$ be continuously differentiable and

$$\mu(x, v; t) = \mu_0(x - X(t), v - V(t))$$

- then μ satisfies

$$\frac{\partial \mu}{\partial t} = \dot{X}^T \nabla_x \mu + \dot{V}^T \nabla_u \mu$$

- eliminate the derivatives of X and V using Newton's equations

$$\frac{\partial \mu}{\partial t} = V \cdot \nabla_x \mu + \frac{F(X, V)}{m} \cdot \nabla_u \mu$$

- **Vlasov equations**

$$\frac{\partial \mu}{\partial t} = v \cdot \nabla_x \mu + \frac{F(x, v)}{m} \cdot \nabla_u \mu$$

approximation if $\text{supp}(\mu_0)$ small

multiple particles

- could use Vlasov equations to define (very) weak solutions of ODEs
- here we consider instead multiple particle solutions given by

$$\mu(x, v; t) = \frac{1}{n} \sum_{i=1}^{n} \mu_0(x - X^{(i)}(t), v - V^{(i)}(t))$$

- if all $(X^{(i)}(t), V^{(i)}(t))$ satisfy Newtons equations one gets the Vlasov approximation as

$$\frac{\partial \mu}{\partial t} = v \cdot \nabla_x \mu + \frac{F(x, v)}{m} \cdot \nabla_u \mu$$

if the forces are purely external, i.e., there are no interactions

multiple particles with interactions

- interactions between the particles: approximate F which now depends on μ

$$\frac{\partial \mu}{\partial t} = v \cdot \nabla_x \mu + \frac{\overline{F}(x, v; \mu)}{m} \cdot \nabla_u \mu$$

- interactions between the particles obtained from the charge and current densities ρ and j

$$\rho_q(x; t) = q \int \mu(x, v; t)\, dv,$$
$$j_q(x; t) = q \int v\mu(x, v)\, dv$$

- nonlinear (quadratic) system of integro-differential equations $\Rightarrow$ turbulence

application and approximation

- the Vlasov equations are used to approximate systems of ODEs arising from very large systems of charged particles
- Vlasov equations are often solved using particle methods which basically model the dynamics of agglomerates of particles
- the accuracy and of the approximations of distributions of discrete particles by densities μ is an area of active research in mathematics especially for the case of Lorentz forces, i.e., the Vlasov-Maxwell equations
- MHD based on moments of μ similar to ρ and j

Approximation 2: gyrokinetics

constant fields

$$m\frac{dv}{dt} = q(E + v \wedge B)$$

- decomposition into terms parallel and orthogonal to B

$$B = (0, 0, |B|)^T$$
$$v = v_{\parallel} + v_{\perp}, \quad E = E_{\parallel} + E_{\perp}$$
$$B \wedge v = |B| \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} v$$

- differential equations for v

$$\frac{dv_{\parallel}}{dt} = \frac{q}{m} E_{\parallel}$$
$$\frac{dv_{\perp}}{dt} = \frac{q}{m} \left(E_{\perp} + v_{\perp} \wedge B \right)$$

solutions of the constant field case

$$v_\parallel(t) = v_\parallel(0) + \frac{qE_\parallel}{m}\, t$$
$$v_\perp(t) = u_\perp + \begin{bmatrix} \cos(\tau) & \sin(\tau) \\ -\sin(\tau) & \cos\tau \end{bmatrix} (v_\perp(0) - u_\perp)$$

where partial (constant) solution $u_\perp$ satisfies $E_\perp + u_\perp \wedge B = 0$ and $\tau = \Omega t$ where the *gyrofrequency* is $\Omega = \frac{q|B|}{m}$

- integrate to get location

$$x_\parallel(t) = x_\parallel(0) + v_\parallel(0)\, t + \frac{qE_\parallel}{m}\,\frac{t^2}{2}$$
$$x_\perp(t) = x_\perp(0) + u_\perp\, t + \Omega \begin{bmatrix} \sin(\tau) & -\cos(\tau) + 1 \\ \cos(\tau) - 1 & \sin(\tau) \end{bmatrix} (v_\perp(0) - u_\perp)$$

discussion of solution

- solution takes the form of a spiral which has two components:
  1. movement of centre
     - in direction of B
     - drifting from this direction
  2. gyration with frequency Ω around centre
- Hamiltonian formulation leads to introduction of gyro coordinates and separation of gyro motion from the rest

invariants and dimension reduction

- Vlasov equations for Hamiltonian systems

$$\frac{\partial f}{\partial t} = \{H, f\}$$

where Poisson bracket is

$$\{H, f\} = \nabla_p H^T \nabla_x f - \nabla_x H^T \nabla_p f$$

- for particles with charge e and $E = \nabla\phi$ and $B = \nabla \wedge A$

$$H = \frac{1}{2m}\|p - \frac{e}{c}A\|^2 + \phi$$

- if $\partial H/\partial x_i = 0$ then Vlasov equations don't contain $\partial f/\partial p_i$ which allows integration

Example

- simple 1D example $H = p^2/2$ then

$$\frac{\partial f}{\partial t} = p f_x$$

  with solution $f = g(pt + x)$
- constant fields with $\phi = E^T x$, $B = \nabla \wedge A$ and Hamiltonian

$$\begin{aligned} H &= \frac{1}{2}\|p - \frac{q}{2c} B \wedge x\|^2 + E^T x \\ &= \frac{1}{2}\left(p_1 + \frac{q|B|}{2c} x_2\right)^2 + \frac{1}{2}\left(p_2 - \frac{q|B|}{2c} x_1\right)^2 + \frac{1}{2} p_3^2 + E_1 x_1 + E_2 x_2 \end{aligned}$$

  - Hamiltonian independent of x_3

Gyrokinetic equations

- approximate one gyrating particle by uniform particle density rotating around gyrocentre
- new coordinates: gyrocentre X, parallel velocity $v_\parallel$ and magnetic moment $\mu = \frac{|mv_\perp|^2}{2B}$ (apologies: different μ ...)
- ODEs (based on Lorentz force)

$$\frac{dX}{dt} = \phi_1(x, v_\parallel, \mu; t)$$
$$\frac{dv_\parallel}{dt} = \phi_2(x, v_\parallel, \mu; t)$$
$$\frac{d\mu}{dt} = 0$$

- Vlasov equations

$$\frac{\partial f}{\partial t} + \phi_1^T \frac{\partial f}{\partial X} + \phi_2 \frac{\partial f}{\partial v_\parallel} = 0$$

- need to transform Maxwell's equations too

Approximation 3: Lie perturbation

Approximating turbulence

- model:

  physical fields = background + turbulent fluctuations
- turbulence smaller than background

$$\frac{\delta f}{f} \text{ and } \frac{\delta B}{B} = O(\epsilon)$$

- time and spatial scales of turbulence larger than gyrations

$$\frac{\omega}{\Omega} \text{ and } \frac{\rho}{L} = O(\epsilon) \quad (\rho\text{: gyroradius, } \Omega\text{: gyrofrequency})$$

- turbulence extends along the magnetic field

$$\frac{k_\parallel}{k_\perp} = O(\epsilon)$$

- Lie perturbation = turbulence perturbation + gyrokinetics

Approximation 4: numerics

geometry and coordinates – fluxtubes

- geometry: torus
- coordinates aligned with magnetic field for efficiency:

$$B \sim \nabla x \wedge \nabla y \quad \text{(Clebsch)}$$

- original GENE (2000) B constant on toroidal surfaces
  - x: radial, z: parallel and y: "poloidal"
  - computation in magnetic fluxtubes with dimensions $\sim$ correlation lengths (long in B direction, short orthogonal)
- current GENE: more general geometry, full 3D domains
- state space = torus $\times$ $\mathbb{R}^2$
  - velocity space approximated by rectangle

discretisation (original local GENE)

- 4th order finite differences on equidistant grid for
  - z with quasiperiodic bnd
  - $v_{\|}$ with Dirichlet bnd $f = 0$
- μ: Gauss-Legendre (or Laguerre) points (required for integral eqn part)
- Fourier spectral method for x and y – use complex computations
- integration in time with fourth order Runge-Kutta

Approximation 5: sparse grids

sparse grid combination technique

- let $h = (h_1, \ldots, h_5)$ be grid sizes of a regular grid approximation f_h in the five dimensions
- choose $h_i \sim 2^{-i}$
- sparse grid combination approximation

$$f_S = \sum_h w_h f_h$$

- use error splitting

$$f_h = f + \sum_\alpha c_\alpha 2^{-\alpha}$$

to obtain error bounds and determine weights w_h

properties and extensions

- optimal choice of w_h give provably smaller errors than any component f_h
- choose w_h such that method is robust against errors
- solving the component problems for f_h provide another dimension of parallelism
- the solutions f appear to be very smooth so that both the sparse grid and the combination technique perform well

quantities of interest

- partial differential equation: find $u \in \mathcal{V}$ such that

$$\mathcal{F}(u) = 0$$

- in our plasma example:
  - $u = (f_1, \ldots, f_k)$ densities $f_s(x, v)$ in state space
  - $\mathcal{F}$ stands for Vlasov-Maxwell equations
- numerical approximation (GENE): find $u_h \in \mathcal{V}_h$ such that

$$\mathcal{F}_h(u_h) = 0$$

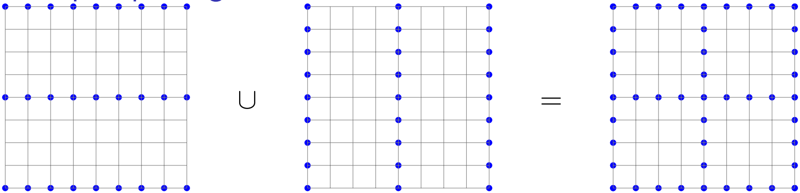
- **quantity of interest**: $q = \mathcal{Q}(u)$
- example

$$\mathcal{Q}(u) = \sum_s m_s \int_\Omega \left| \int_{\mathbb{R}^3} v\, f_s(x, v)\, dv \right|^2 \, dx$$

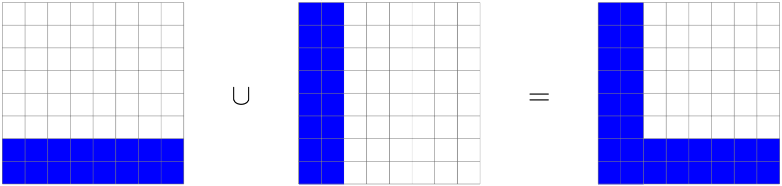
- approximation (GENE): $q_h = \mathcal{Q}_h(u_h)$

a sparse grid

a simple sparse grid



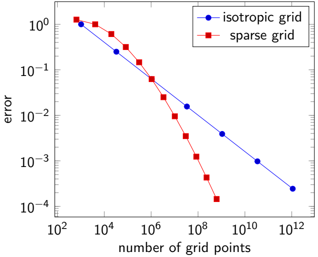
sparse grid in frequency / scale space



captures fine scales in both dimensions but not joint fine scales

sparse grid error

five dimensional case



- only asymptotic error rates given here
- constants and preasymptotics also depend on dimension
- practical experience: with sparse grids up to 10 dimensions
- Zenger 1991

asymptotic rates	number of points	L_2 error
regular isotropic grids	h^{-d}	h^2
sparse grids	$h^{-1}\,\lvert\log_2 h\rvert^{d-1}$	$h^2\,\lvert\log_2 h\rvert^{d-1}$

combination technique

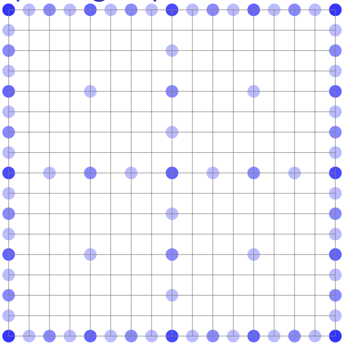
- compute combination coefficients using exclusion-inclusion principle
- u_h approximations of u, $h = (h_1, h_2, \ldots) = (2^{-\gamma_1}, 2^{-\gamma_2}, \ldots)$ size of grid cells
- u_{SG} sparse grid approximation
- u_C combination approximation
- examples: interpolation, best approximation, Galerkin solution of PDE, other PDE solvers
- if the approximations for any two discretisations commute, then the sparse grid approximation is equal to the combination approximation – example: interpolation
- error-splitting formulas replace Euler-Maclaurin:

  $$u_h - u = \beta_1 h_1^2 + \beta_2 h_2^2 + \beta_3 h_1^2 h_2^2 + \cdots$$

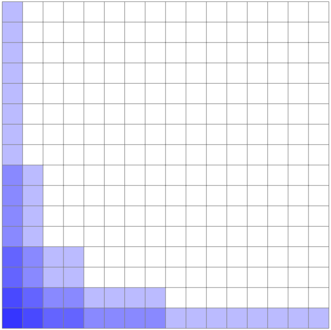
  only available for simple cases (Laplace equation etc)
- study of the surplus for wider range of cases suggests that error splitting holds more widely

combination formula

sparse grid points



sparse grid scale diagram



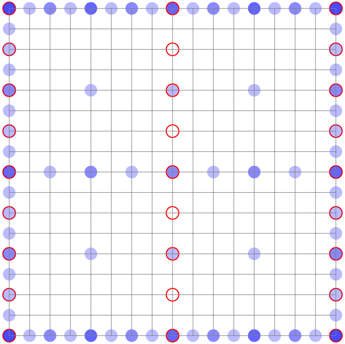
combination formula

$$u_C = u_{1,16} + u_{2,8} + u_{4,4} + u_{8,2} + u_{16,1} - u_{1,8} - u_{2,4} - u_{4,2} - u_{8,1}$$

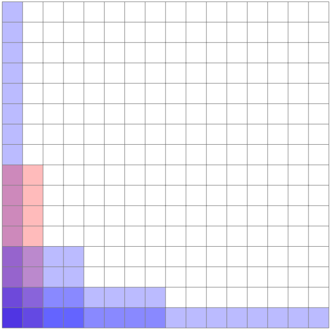
Griebel, Schneider, Zenger 1992

fault tolerant sparse grids

sparse grid points



sparse grid scale diagram



revised combination formula

$$u_C = u_{1,16} + u_{4,4} + u_{8,2} + u_{16,1} - u_{4,2} - u_{8,1} - u_{1,4}$$

H. CTAC 2003, Harding 2012

Other approximations

examples

- Strang splitting
- MHD
- SPH – particle methods, meshless methods
- discontinuous Galerkin
- reduced basis methods

References

- Jenko et all 2000: first GENE paper
- Tobias Goerler, PhD thesis, 2009 (GENE)
- Neunzert/Wick 1974 (ODEs)
- Braun-Hepp 1977 (ODEs)
- Lazarovici 2018 (ODEs)
- Brizard/Hahm 2006 (gyrokinetics, Lie perturbation)
- Beer/Cowley/Hammett 1995 (field-aligned coordinates)
- various papers by Kowitz, Harding, Jenko, Pfluger and H. (sparse grids and GENE) in last 10 years