Block-Structured Grids in Gyrokinetic Plasma Simulation

Tobias Neckel
**Plasma - 4th State of Matter**

**Plasma** – fourth state of matter, electrically quasi-neutral medium of unbound positive and negative charges

**Plasma condition:**
- **Coulomb energy** << **Kinetic energy**

Motivation

• Why is plasma simulation interesting?
  – Understanding various phenomena
  – Support layout of fusion reactors

• Challenges: Turbulence effects
  ⇒ massive temperature losses
  ⇒ mandatory to reduce/optimize losses
Motivation

- Why is plasma simulation interesting?
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- Challenges: Turbulence effects
  - Massive temperature losses
  - Mandatory to reduce/optimize losses

- Simulation: crucial + expensive!
- Different approaches for plasma sims
  - Here: gyrokinetics
Motivation

Code Platform for Simulations: GENE

- ~10 developers, ~O(100) users
- FORTRAN
- Parallel: up to 262,144 cores
- Typical production run:
  #CPUs: 8,000-32,000
  #CPU hours: ~10 million
  #DoF: up to 10 billion

GENE
Gyrokinetic Electromagnetic Numerical Experiment
http://genecode.org
Motivation

• Collaborators
  - Frank Jenko & group (MPP, now UCLA)
  - Denis Jarema (TUM)

• Projects: **HEPP** & **G8 Nu-FuSe** & **SPPEXA**
  - adaptivity & grids
  - numerical lin. algebra (eigenvalue solvers, PC)
  - resilience via sparse grids
Motivation and Goals

Motivation:
- global GENE simulations: computationally expensive
- regular grids: not always an optimal choice :-)

Goal:
- adaptive meshes in GENE
  ⇒ enhance performance without losing accuracy

Side conditions:
- keep (complex) physical discretisations (tight coupling)
- keep interfaces, use of data structures, etc. for users/developers
Outline

• Motivation & Intro

• GENE Simulations
  ▪ Governing Equation
  ▪ Discretization

• Block-Structured Grids
  ▪ Construction
  ▪ Parallelization

• Simulations Results
  ▪ Linear Simulations
  ▪ Nonlinear Simulations

• Summary & Outlook
Towards Gyrokinetics

**GENE**: based on gyrokinetic theory

- **Kinetic**: reduce dimension: 6
- **Gyro-kinetic**: reduce dimension: 5

![Diagram showing reduction in dimension from 6 to 5](image-url)
Towards Gyrokinetics

Gyrokinetics – Governing Equations

Vlasov-Maxwell Equations

Vlasov:
\[
\frac{\partial F_s}{\partial t} + \mathbf{X} \cdot \nabla F_s + \mu \frac{\partial F_s}{\partial \mu} + \dot{v}_\parallel \frac{\partial F_s}{\partial v_{\parallel}} = 0
\]

Maxwell:
\[
-\nabla^2 \Phi_1 = 4\pi \sum_s q_s \int d^3v F_s \\
-\nabla^2 A_1 = \frac{4\pi}{c} \sum_s q_s \int d^3v v F_s
\]

Splitting:
\[
F_s = F_{0s} + f_{1s} \quad \frac{f_{1s}}{F_{0s}} \ll 1
\]

\[\rightarrow\text{non-lin. 5D partial integro-differential system for particle density fluctuation} \quad f_{1s}(x, y, z, v_{\parallel}, \mu)\]
Structure of Governing Equation

Time derivative of distribution function

= \text{drive term} + \text{nonlinearity (ExB drift)} + \text{curvature term} + \ldots

= \text{pressure term} + \text{parallel dynamics} + \text{trapping term} + \ldots

for n grid points:
Linear part: complexity $\sim O(n)$
Nonlinear part: complexity $\sim O(n \log(n))$

New grid in GENE = new implementation of rhs for governing equation + new initialization routines
5D Phase Space Discretisation: Grids & Ops

- **Radial direction x:** config./Fourier space
- **Toroidal direction y:** Fourier space
- **Parallel direction z:** configuration space
- **Parallel velocity v_∥:** configuration space
- **Magnetic moment µ:** Gauss-Laguerre points
- **Time discretisation:** explicit Runge-Kutta (non-standard)

Source: T. Görler. Multiscale Effects in Plasma Microturbulence
Local and Global Regimes

Local in radial direction
- Small simulation domain if $\rho^* = \rho_s/a \ll 1$ and small profile variation
- Periodic boundary conditions (BC) – spectral methods

Global
- Full temperature and density profiles
- Dirichlet or Neumann BC – finite differences in radial direction
Examples of Temperature and Density Profiles

Background distribution function:

\[ F_0 \left( x, v^\parallel, v^\perp x, v^\perp y \right) = \frac{n(x)}{\pi^{3/2} v^3_T(x)} \exp \left[ -\frac{mv^2_\parallel/2 + \mu B}{T(x)} \right]. \]
Projections of Background Distribution Function

Projection on parallel velocity – radial distance space

Projection on magnetic moment – radial distance space
Structure of Existing Regular Grids

Projection on parallel velocity – radial distance space
Structure of Existing Regular Grids

Two local grids in parallel velocity – radial distance space

Resulting regular grid
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First Type Block-Structured Grids
Parallel Velocity – Radial Coordinate Space

Projection on parallel velocity – radial distance space

Corresponding grid in parallel velocity – radial distance space
First Type Block-Structured Grids
Magnetic Moment – Radial Coordinate Space

Projection on magnetic moment – radial distance space

Corresponding grid in magnetic moment – radial distance space
Reduction of Grid Points in First Type Block-Structured Grids

- # blocks: 4
- # points in regular grid: 100% (nx0=512, nv0=96, nw0=64)
- # points in $v_{||}$-x (BS) grid: 73%
- # points in $\mu$-x (BS) grid: 79%
- # points in $v_{||}$-$\mu$-x (BS) grid: 64%
Second Type Block-Structured Grids
Parallel Velocity – Radial Coordinate Space

Two local grids in parallel velocity – radial distance space

Resulting regular grid
Reduction of Grid Points in 2\textsuperscript{nd} Type Block-Structured Grids

\begin{itemize}
  \item \# blocks: 4
  \item \# points in regular grid: 100\% (nx0=512, nv0=96, nw0=64)
  \item \# points in $v \parallel -x$ (BS) grid: 42\% 
  \item \# points in $\mu - x$ (BS) grid: 79\% 
  \item \# points in $v \parallel -\mu - x$ (BS) grid: 33\%
\end{itemize}
Number of Grid Points in Block-Structured Grids

Number of grid points in 2\textsuperscript{nd} type block-structured grid
(based on regular grid: nx0=512, nv0=96, nw0=64)
Treatment of Block Boundaries

- \( \times \) derivative computation node
- \( \bullet \) nodes directly used in stencil computations
- \( \Delta \) pseudo-nodes with interpolated values
- \( \square \) nodes used for interpolation

boundary between blocks
Parallelisation of Block-Structured Grids

- Processes grid boundary
- Grid coordinate lines
- Vertical exchange
- Side exchange
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Examples of Fluctuating Parts $f_1$ of Distribution Function for Linear Simulations

TCV electrons profile simulations with one species

Analytical profile simulations with two species (fluctuating part for electrons)
Results of Linear Simulations: TCV: Convergence Curves for Regular and Block-Structured Grids

<table>
<thead>
<tr>
<th>grid type</th>
<th>regular</th>
<th>BS 1</th>
<th>BS 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>nv0</td>
<td>96</td>
<td>96</td>
<td>36</td>
</tr>
<tr>
<td>γ</td>
<td>0.371</td>
<td>0.371</td>
<td>0.357</td>
</tr>
<tr>
<td>ω</td>
<td>-0.056</td>
<td>-0.056</td>
<td>-0.050</td>
</tr>
<tr>
<td>steps</td>
<td>35359</td>
<td>35359</td>
<td>7779</td>
</tr>
<tr>
<td>Δt (s)</td>
<td>0.808</td>
<td>0.521</td>
<td>0.390</td>
</tr>
<tr>
<td>time (s)</td>
<td>28577</td>
<td>18415</td>
<td>3035</td>
</tr>
<tr>
<td>speedup</td>
<td>-</td>
<td>1.6</td>
<td>9.4</td>
</tr>
</tbody>
</table>

γ – growth rate, ω – frequency

BS2 converges (accuracy 1e-3) at nv0 ~ 70, regular grid at nv0 ~ 96 (nx0=512, nz0=16, nw0=64)
Results of Linear Simulations: Convergence Curves for Regular and Second Type Block-Structured Grids

BS2 converges (accuracy $1e^{-3}$) at $nv_0 = 100$, regular grid at $nv_0 = 260$ ($nx_0=256$, $nz_0=16$, $nw_0=64$)
Nonlinear Simulations: Experiment Description

regular grid: reference grid with wide range, fine resolution

block-structured grid: blocks of regular grid adapted to background distribution

1st alternative regular grid: grid with wide range, coarse resolution

2nd alternative regular grid: grid with narrow range, fine resolution
Results of Nonlinear Simulations:
Time-averaged Fluctuating Part $f_1$ of Distribution Function

Time-average fluctuating part $f_1$ of distribution function for regular reference grid

Speedup: 1.9 – 3.0

Plots over line at fixed $v_\parallel = 0$ for four different computational grids
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Summary

- Adaptivity via block-structured grids
- Considerable performance enhancements
- No accuracy losses
- Keep structure/design of legacy code
Outlook

- 2\textsuperscript{nd} type block-structured grids:
  in magnetic moment – radial distance space
- Extend GENE: support different block-structured grids for different species
- Work on performance optimization of block-structured grids
Magnetic Moment Direction – Gauss Laguerre Integration

The usual fluid moments like density, average fluid velocity and temperature are defined in terms of the total particle distribution.

\[ n_j(x) = \int F_j(x,v) \, d^3v \]
\[ u_j(x) = \frac{1}{n_j(x)} \int v F_j(x,v) \, d^3v \]
\[ T_j(x) = \frac{1}{n_j(x)} \int \frac{m}{2} (v - u_j)^2 F_j(x,v) \, d^3v. \]

Classical Gauss-Laguerre quadrature:
\[
\int_0^\infty e^{-(\lambda=1)x} f(x) \, dx = \sum_{i=1}^{n} \omega_i f(x_i)
\]

Blocking (changing ranges) = adjusting quadrature to different \( \lambda \)

\[
\int_0^\infty e^{-\lambda \mu} f(\mu) \, d\mu = \frac{1}{\lambda} \int_0^\infty e^{-x} f(x) \, dx = \sum_{i=1}^{n} \omega_i x_i f(x_i) = \sum_{i=1}^{n} \omega_i^\lambda f(\mu_i),
\]

New nodes and weights: \( \mu_i = x_i / \lambda, \quad \omega_i^\lambda = \omega_i / \lambda \)
Second Type Block-Structured Grids
Magnetic Moment – Radial Coordinate Space

Integration of $F_0$ with different Gauss-Laguerre quadrature rules

- $nw0=4$
- $nw0=16$
- $nw0=8$
- $nw0=32$
Second Type Block-Structured Grids
Magnetic Moment – Radial Coordinate Space

Projection of fluctuating part $f_1$ of distribution function on magnetic moment – radial distance space
References


Thanks for your attention!