Recent developments in the theory and application of the sparse grid combination technique

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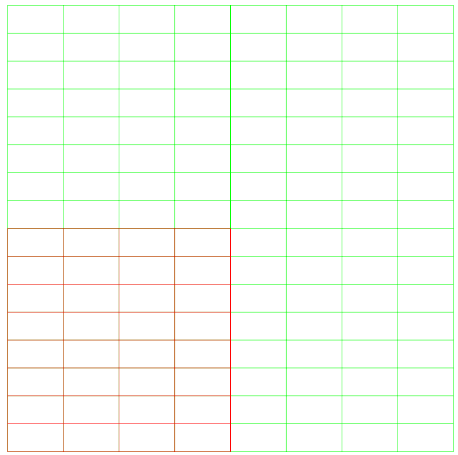
Section 1

Overview

Basic extrapolation approach

- use a highly scalable PDE solver
- run for a selection of numerical grids
- combine results to get higher accuracy and fault tolerance

spatial discretisation



- $n_1 \times n_2$ grid with $n_i = 2^{\gamma_i} + 1$, e.g. $\gamma = (3, 4)$
- parallelise over cells of size $m_1 \times m_2$, e.g. $m_{1,2} = 5, 9$
- numerical solution $u(\gamma)(x, t)$ obtained by interpolation

The PDE: Vlasov–Maxwell Equations

- Vlasov-Equation

$$\frac{\partial f_s}{\partial t} + \vec{v} \cdot \frac{\partial f_s}{\partial \vec{x}} + \frac{q_s}{m_s}(\vec{E} + \vec{v} \times \vec{B}) \cdot \frac{\partial f_s}{\partial \vec{v}} = 0$$

- Moments of the Distribution Function f

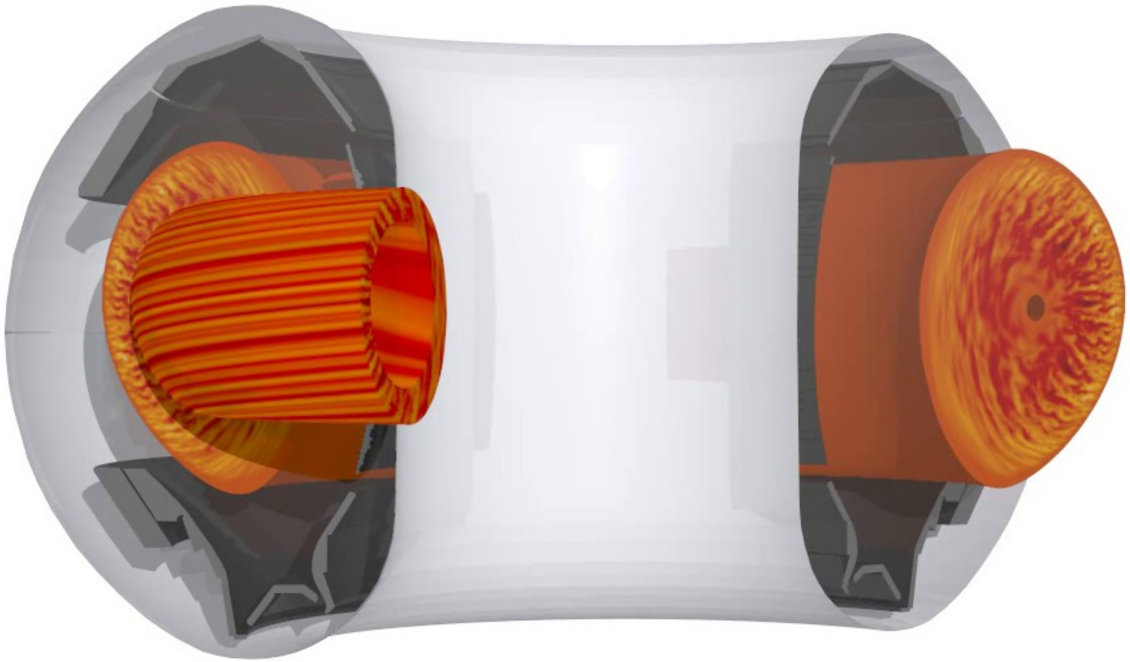
$$\rho(\vec{x}, t) = \sum_s q_s \int f_s(\vec{x}, \vec{v}, t)\, dv \quad \vec{j}(\vec{x}, t) = \sum_s q_s \int f_s(\vec{x}, \vec{v}, t)\vec{v} dv$$

- Maxwell Equations

$$-\frac{1}{c^2}\frac{\partial \vec{E}}{\partial t} + \nabla \times \vec{B} = \mu_0(\vec{j}_0 + \vec{j}) \qquad \nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}$$

$$\frac{\partial \vec{B}}{\partial t} + \nabla \times \vec{E} = 0 \qquad \nabla \cdot \vec{B} = 0$$

GENE – Gyrokinetic Electromagnetic Numerical Experiment (genecode.org)



- open source plasma research code for investigation of microturbulence
- gyrokinetic approximation of the Vlasov equations
- nonlinear parametrisation of state space with 5 dimensions
- uses MPI and has been shown to be strongly scalable

Section 2

Sparse grid combination technique

Hierarchical decomposition

- let V_γ be the approximation space corresponding to $u(\gamma)$
- we assume $V_\alpha \subset V_\beta$ if $\alpha \leq \beta$
- hierarchical decomposition of $u(\gamma) \in V_\gamma$ into $w(\alpha) \in V_\alpha$:

  $$u(\gamma) = \sum_{\alpha \leq \gamma} w(\alpha)$$

  such $w(\alpha)$ exist and are unique, there is a formula ...
- if $u(\gamma) = I_\gamma u$ are the interpolants in V_γ on regular grids, the $w(\alpha)$ are the *hierarchical surplus* of u in V_α

Motivation for the decomposition

- in some cases

$$\|w(\alpha)\| \leq K4^{-|\alpha|}$$

  where $|\alpha| = \alpha_1 + \cdots + \alpha_d$
- the values of $4^{-|\alpha|}$ for $\alpha \leq (5,5)$ are

10^{-3}	$2.5 \cdot 10^{-4}$	$6 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$	$4 \cdot 10^{-6}$	10^{-6}
$4 \cdot 10^{-3}$	10^{-3}	$2.5 \cdot 10^{-4}$	$6 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$	$4 \cdot 10^{-6}$
0.016	$4 \cdot 10^{-3}$	10^{-3}	$2.5 \cdot 10^{-4}$	$6 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$
0.0625	0.016	$4 \cdot 10^{-3}$	10^{-3}	$2.5 \cdot 10^{-4}$	$6 \cdot 10^{-5}$
0.25	0.0625	0.016	$4 \cdot 10^{-3}$	10^{-3}	$2.5 \cdot 10^{-4}$
1	0.25	0.0625	0.016	$4 \cdot 10^{-3}$	10^{-3}

- typical complexity of computing $w(\alpha)$ is $O(2^{|\alpha|})$ – the smallest components are the most expensive:
  - $w(5,5)$ costs 1024 times more than $w(0,0)$
  - neglecting $w(5,5)$ produces error in sixth digit

Motivation for the decomposition

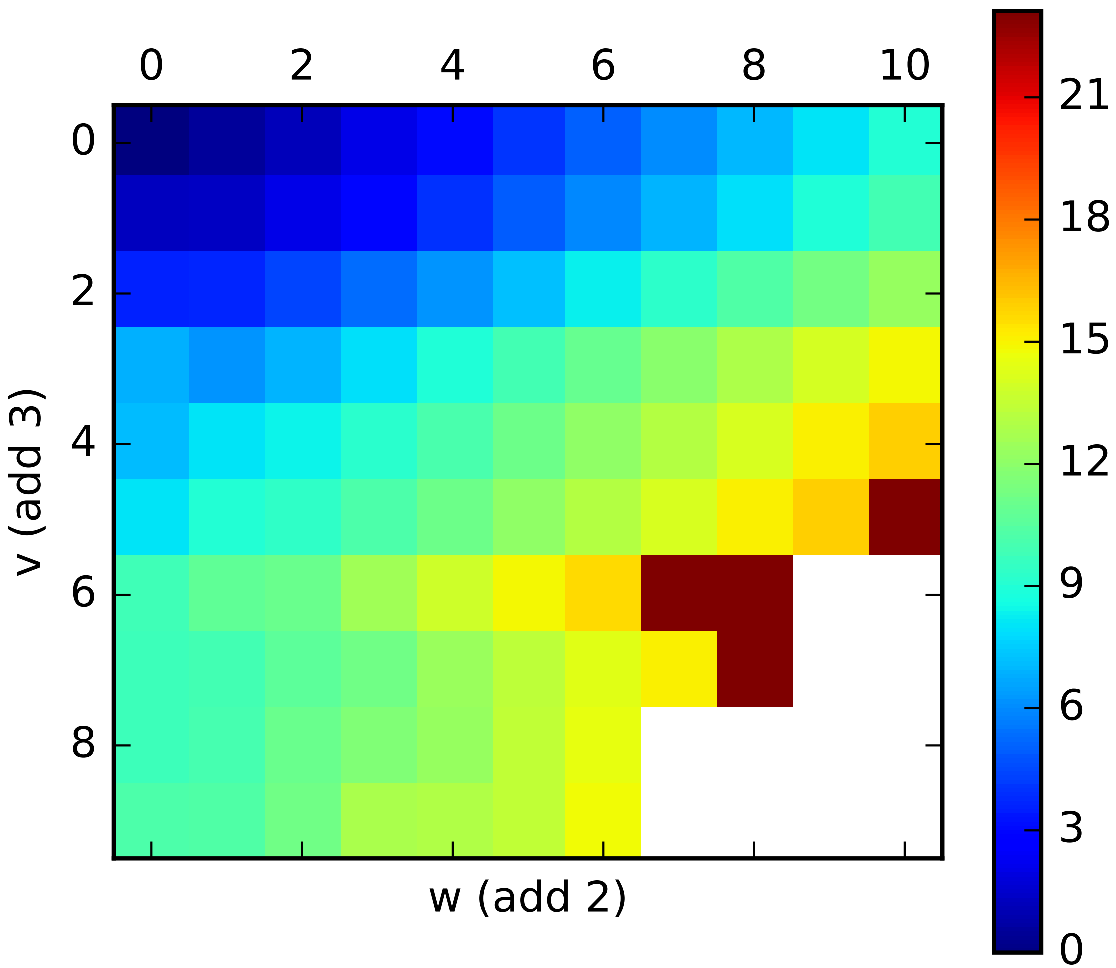


Figure 1:surplus of QoI

Combination formula

- sparse grid combination approximation of $u(\gamma)$ for $\gamma = (n, n, \dots, n)$

$$u_n^C = \sum_{|\alpha| \leq n} w(\alpha)$$

- combination formula[1]

$$u_n^C = \sum_{|\gamma| \leq n} c_\gamma \, u(\gamma)$$

- in the case of $n = 2$ and $d = 2$ this is

$$u_2^C = u(0,2) + u(1,1) + u(2,0) - u(0,1) - u(1,0)$$

[1] $|\alpha| = \alpha_1 + \cdots + \alpha_d$

Sketch of parallel performance

1. Compute all component solutions $u(\gamma)$
   - computation of every component is distributed over subcluster[2]
   - multiple $u(\gamma)$ are computed concurrently
   - lower bound for wall clock time $O(2^n/p)$
2. Compute the combination $\sum_\gamma c_\gamma \, u(\gamma)$
   - distributed addition of one component to the sum
   - parallel summation
   - lower bound for wall clock time $O((d-1)\log_2(n)\, 2^n/p)$

For PDE solvers, time for first step usually dominates

[2] $p=$ size of subcluster

Section 3

nonstandard sparse grids

When some components $u(\gamma)$ are missing

- large errors (predicted or detected) in $u(\gamma)$ because of limitations of physical model, numerical approximation or faults
  - error detection may use the $w(\alpha)$
- components $u(\gamma)$ have not been computed due to hardware issues
- some components $w(\alpha)$ are predicted to be very small and can be neglected

approach

- determine downset containing available grids
- compute some of the missing ones
- use combination coefficients for the particular downset

when a top level component is missing

- case of $n = 5$ and $d = 2$ (target grid: blue)

$(0,5)$					$(5,5)$
$(0,4)$	$(1,4)$				
	$(1,3)$	$(2,3)$			
	$(1,2)$	$(2,2)$	$(3,2)$		
			$(3,1)$	$(4,1)$	
				$(4,0)$	$(5,0)$

- the error increases by $w(2,3)$ if $u(2,3)$ is missing (yellow)
- we need to compute $u(1,2)$ in order to compute this approximation (red)
- the values $u(1,3)$ and $u(2,2)$ are now not needed any more (green)
- solution: compute all components 2 levels down from the top (this is cheap as the corresponding grids are small)

when a component at a lower level is missing

- case of $n = 5$ and $d = 2$ (target grid: blue)

$(0,5)$					$(5,5)$
$(0,4)$	$(1,4)$				
	$(1,3)$	$(2,3)$			
	$(1,2)$	$(2,2)$	$(3,2)$		
			$(3,1)$	$(4,1)$	
				$(4,0)$	$(5,0)$

- when $u(2,2)$ is missing (yellow) we again could compute $u(1,2)$ (red)
- in the combination one then does not use $u(1,3)$ and $u(2,3)$ (green) and the error increases by $w(2,3)$
- two possible solutions:
  - precompute the components two levels down from the top
  - duplicate computations of all components one level from the top

Families of sparse grids for the combination technique

$$u_I = \sum_{\gamma \in I} c_\gamma \, u(\gamma)$$

- classical SG: $I = \{\alpha \mid |\alpha| \leq n + d - 1\}$
- truncated SG[3]: $I = \downarrow \{\alpha \mid |\alpha| \leq n + d - 1, \ \alpha \geq \beta\}$
- partial SG if $\beta \geq 1$:
  $$I = \downarrow \{\alpha \mid |\alpha| \leq n + |\beta| - 1, \ \alpha \geq \beta\}$$
- SG if $u(\beta)$ removed and $|\beta| = n + d - 1$:
  $$I = \{\alpha \mid |\alpha| \leq n + d - 1, \ \alpha \neq \beta\}$$
- 2-scale SG[4]:
  $$I = \bigcup_{k=1}^{d} \{\alpha \mid \alpha \leq n_0 1 + n_k e_k\}$$
- ANOVA:
  $$I = \{\alpha \mid |\operatorname{supp} \alpha| \leq k\}$$

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[3] $\downarrow I$ is smallest downset containing I

[4] special case: $n_0 = n_k = n$

Section 4

nonstandard coefficients

Opticom method – best possible combination coefficients

- convex optimisation problem

$$u = \operatorname{argmin}\{J(v) \mid v \in V\}$$

- Ritz method

$$u(\gamma) = \operatorname{argmin}\{J(v) \mid v \in V(\gamma)\}$$

- Opticom method utilises Ritz approach

$$u^O = \operatorname{argmin}_v\{J(v) \mid v = \sum_{\gamma \in I} c_\gamma u(\gamma),\ c_\gamma \in \mathbb{R}\}$$

- Ritz is quasi optimal for appropriate norm

$$\|u^O - u\| \leq C \left\| \sum_\gamma c_\gamma u(\gamma) - u \right\| \quad \text{for all } c_\gamma \in \mathbb{R}$$

Comparing a general combination with the standard one for classical sparse grid

$$
\begin{aligned}
u_n^C - u_n^{SG} &= \sum_{|\gamma|\le n} c_\gamma u(\gamma) - \sum_{|\alpha|\le n} w(\alpha) \\
&= \sum_{|\gamma|\le n} c_\gamma \sum_{\alpha\le\gamma} w(\alpha) - \sum_{|\alpha|\le n} w(\alpha) \\
&= \sum_{|\alpha|\le n} \left(\sum_{\gamma\in I(\alpha,n)} c_\gamma - 1 \right) w(\alpha)
\end{aligned}
$$

where $I(\alpha, n) = \{\gamma \mid |\gamma| \le n, \alpha \le \gamma\}$

- bracket is zero for standard sparse grid solution
- faults require to set certain c_γ to zero

An optimal apriori choice of the (remaining) c_γ

- for the case where $u(\beta)$ is not available or not acceptable one sets $c_\beta = 0$ and the other components are obtained minimising $J(\mathbf{c})$:

$$\mathbf{c}^{\text{best}} = \operatorname{argmin}\{J(\mathbf{c}) \mid c_\beta = 0\}$$

  where $\mathbf{c}$ is the vector with components c_γ for $|\gamma| \le n$ and

$$J(\mathbf{c}) = \sum_{|\alpha| \le n} 4^{-|\alpha|} \left| \sum_{\gamma \in I(\alpha, n)} c_\gamma - 1 \right|$$

  this is a piecewise linear optimisation problem with constraints
- the form of the objective function is motivated by the bounds

$$\|w(\alpha)\| \le 4^{-|\alpha|} K$$

- approximation error is then bounded by

$$\|u_n^C - u_n^{\text{SG}}\| \le K\, J(\mathbf{c})$$

Section 5

Application

Eigenvalue problems

- eigenvalue problem $Lu = \lambda u$ with constraint $\langle s, u \rangle = 1$
- let $u(\gamma)$ and $\lambda(\gamma)$ be approximations satisfying the constraint
- introduce the operator $G : \mathbb{R}^m \to V$ defined by

$$Gc = \sum_{\gamma \in I} c_\gamma \, u(\gamma)$$

- consider the quadratic optimisation problem

$$(c^C, \lambda^C) = \operatorname{argmin}_{(c,\lambda)} \|LGc - \lambda Gc\|$$

with constraint[5] $\sum_{\gamma \in I} c_\gamma = 1$

[5] follows from the constraint $\langle s, Gc \rangle = 1$

A solution from 1964

- Osborne considered the problem

$$\begin{bmatrix} K(\lambda) & t \\ s^* & 0 \end{bmatrix} \begin{bmatrix} c \\ \beta \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- this gives

$$\beta(\lambda) = -\frac{1}{\langle s^*, K(\lambda)^{-1} t \rangle}$$

- the problem $\beta(\lambda) = 1$ is then solved with Newton's method
- application to the combination technique with

$$K(\lambda) = (LG - \lambda G)^* (LG - \lambda G)$$

- thus we get the method:
  1. solve the component problems to get $u(\gamma)$
  2. reduction operation to compute the matrix $K(\lambda)$
  3. solve the optimisation problem to get the coefficients c_γ
  4. evaluate the combination $\sum_{\gamma \in I} c_\gamma u(\gamma)$

Summary

- consider general combination formulas of the form

$$u^C = \sum_{\gamma \in I} c_\gamma u(\gamma)$$

- theory based on hierarchical decompositions

$$u(\gamma) = \sum_{\alpha \leq \gamma} w(\alpha)$$

- lead to new algorithms
  - with extra degree of parallelism
  - avoids curse of dimension
  - provides a new level of fault tolerance
  - maintains scalability
  - reuses the original code to compute $u(\gamma)$