

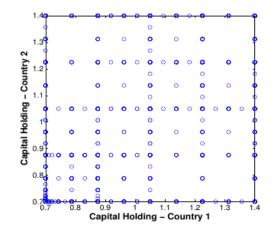


### **Sparse Grids**

### Simon Scheidegger

ZICE, University of Zürich, Jan 31st 2017

Brumm & Scheidegger (2014)
Preprint: http://papers.ssrn.com/sol3/papers.cfm?abstract\_id=2349281





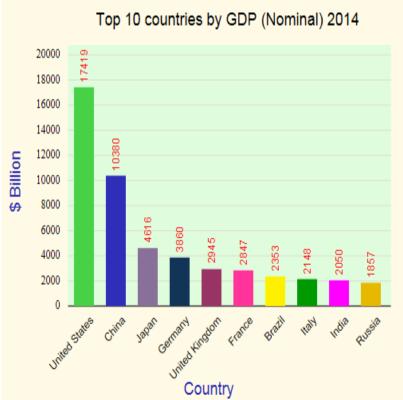
# **Outline**

- Motivation "the curse of dimensionality"
- II. From Full (Cartesian) Grids to Sparse Grids
- III. Adaptive Sparse Grids
- IV. Putting things together: Time Iteration, Adaptive Sparse Grids & High-Performance Computing (HPC)

### Example – Heterogeneity in IRBC models

- Model trade imbalance
- FX rates

-...





- How many regions does a minimal model have?
- Are policy functions smooth? (borrowing constraints)
- → Model heterogeneous & high-dimensional

### Example – Heterogeneity in OLG\* models

\*Overlapping generation models



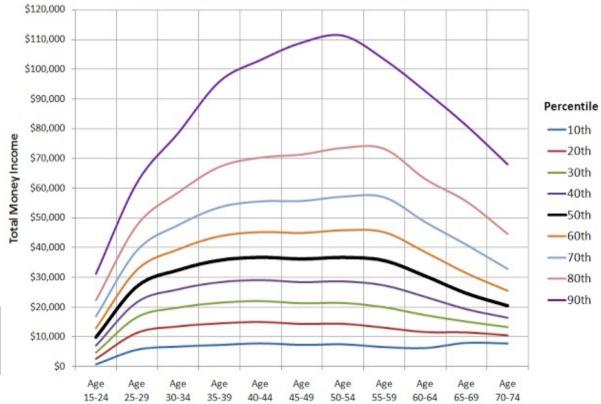
To model e.g. social security:

- How many age groups?
- borrowing constraints?
- aggregate shocks?

- ...

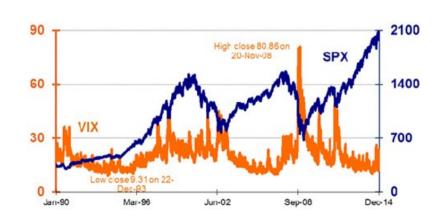
→ Model: heterogeneous & high-dimensional





# Financial markets: non-Gaussian returns

- Derivative contracts giving a right to buy or sell an underlying security.
  - European if exercise at expiration only.
  - American if exercise any time until expiration.
- American options are <u>extremely challenging</u>:
  - → Dynamic optimization problem.
- Basic models do not describe dynamics accurately (e.g., Hull (2011)).
- Financial returns are often not Gaussian.
- Realistic models are hard to deal with, as they need many factors.
  - → Curse of dimensionality.



### Dynamic Programming/Value Function Iteration

e.g. Stokey, Lucas & Prescott (1989), Judd (1998), ...

Dynamic programming seeks a time-invariant policy function  $\boldsymbol{p}$  mapping a state  $\mathbf{x}_t$  into the control  $\mathbf{u}_t$  such that for all  $t \in \mathbb{N}$   $u_t = p(x_t)$  The solution is approached in the limit as  $j \to \infty$  by iterations on:

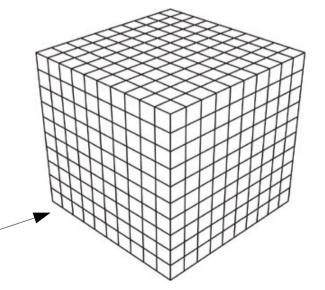
$$V_{j+1} \underline{(x)} = \max_{u} \{ r\left(x, u\right) + \beta V_{j}\left(\tilde{x}\right) \}$$
 s.t. 
$$\tilde{x} = g(x, u)$$

x: grid point, describes your system. State-space potentially high-dimensional.

`old solution':

high-dimensional function on which we interpolate.

- $\rightarrow$  N<sup>d</sup> points in ordinary discretization schemes.
- → Use-case for (adaptive) sparse grids.



### How many is dimensions is high dimensions?



I. Motivation

### How many is dimensions is high dimensions?

Number of parameters (the dimension)	Number of model runs (at 10 points per dimension)	Time for parameter study (at 1 second per run)
1	10	10 sec
2	100	~ 1.6 min
3	1,000	~ 16 min
4	10,000	~ 2.7 hours
5	100,000	~ 1.1 days
6	1,000,000	~ 1.6 weeks
20	1e20	3 trillion years (240x age of the universe)

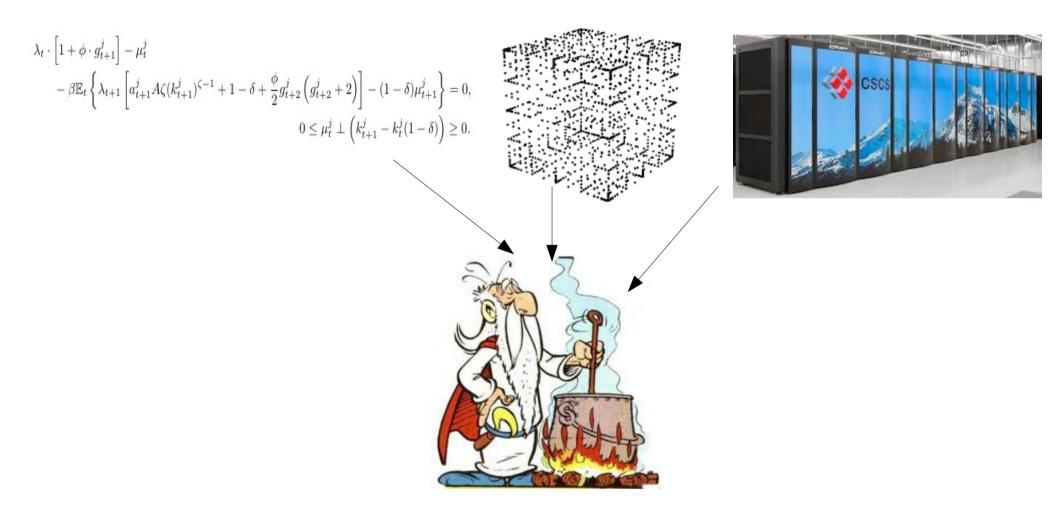
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Dimension reduction Exploit symmetries,	Deal with #Points  Adaptive Sparse Grids	High-performance computing Reduces time to solution, but not the problem size

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# Computational modelling



## **Abstract Problem Formulation**

i) Dynamic models: heterogeneous & high-dimensional

ii) Want to solve dynamic stochastic models with high-dimensional state spaces

→ Have to approximate and interpolate high-dimensional functions

Problem: curse of dimensionality

- → N<sup>d</sup> points in ordinary discretization schemes
- iii) Want to overcome curse of dimensionality
- iv) Want locality & adaptivity of interpolation scheme
- v) Speed-up → access hybrid HPC systems (MPI, OpenMP, TBB, GPU)

### Models where high-dim. state spaces show up

e.g. Stokey, Lucas & Prescott (1989), Ljundquist & Sargent (2004), Krüger & Kübler (2004), Judd et. al. (2013),...

- •International Real Business Cycle (IRBC) Models: **Exchange Rates, Global Trade Imbalances**
- Dynamic Stochastic General Equilibrium (DSGE) Models:
   Monetary Policy, Business Cycle Fluctuations
- Overlapping Generations (OLG) Models:
   Demographic Change, Social Security
- Mathematical Finance:Option pricing,...

## **Our Method**

#### **Adaptive Sparse Grids:**

- Alleviate curse of dimensionality by sparsity.
- Capture non-smoothness by adaptivity.

#### Dynamic Programming (DP) / Time iteration:

- Iteratively update e.g. value functions or policy functions.

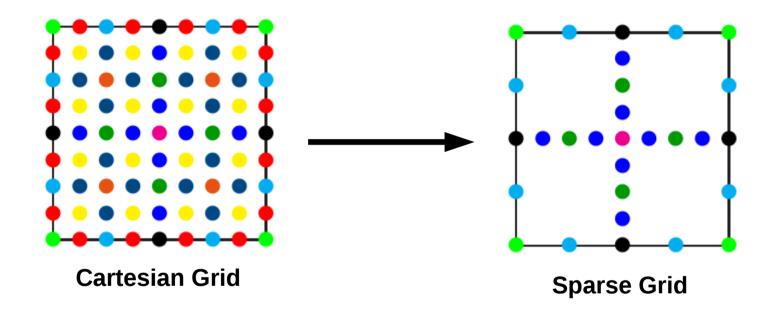
#### **High-Performance Computing:**

- Achieve massive speed-up by efficiently using modern supercomputers with hybrid parallelization scheme.

#### ⇒ Parallel DP Adaptive-Sparse-Grid Algorithm

# **II. From Full Grids to Sparse Grids**

(see, e.g. Zenger (1991), Bungartz & Griebel (2004), Garcke (2012), Pflüger (2010),...)



# Interpolation on a Full Grid

- -Consider a 1-dimensional function  $f:\Omega\to\mathbb{R}$  on [0,1]
- -In numerical simulations:
- f might be expensive to evaluate! (solve PDEs/system of non-linear Eqs.) But: need to be able to evaluate f at arbitrary points using a numerical code
- -Construct an interpolant  $\mathbf{u}$  of  $\mathbf{f}$   $f(\vec{x}) \approx u(\vec{x}) := \sum_{i} \alpha_{i} \varphi_{i}(\vec{x})$
- -With suitable basis functions:  $\varphi_i(\vec{x})$  and coefficients:  $\alpha_i$
- For simplicity: focus on case where  $f|_{\partial\Omega}=0$

### **Basis Functions**

-Hierarchical basis based on hat functions

$$\phi(x) = \begin{cases} 1 - |x| & \text{if } x \in [-1, 1] \\ 0 & \text{else} \end{cases}$$

-Used to generate a **family of basis functions**  $\phi_{l,i}$  having support  $[x_{l,i} - h_l, x_{l,i} + h_l]$  by **dilation** and **translation** 

$$\phi_{l,i}(x) := \phi\left(\frac{x - i \cdot h_l}{h_l}\right)$$

# Hierarchical Increment Spaces

#### **Hierarchical increment spaces:**

$$W_l := \operatorname{span}\{\phi_{l,i} : i \in I_l\}$$

with the index set

$$I_l = \{i \in \mathbb{N}, 1 \le i \le 2^l - 1, i \text{ odd}\}$$

The corresponding function space:

$$V_l = \bigoplus_{k \le l} W_k$$

#### The 1d-interpolant:

$$f(x) \approx u(x) = \sum_{k=1}^{l} \sum_{i \in I_k} \alpha_{k,i} \phi_{k,i}(x)$$

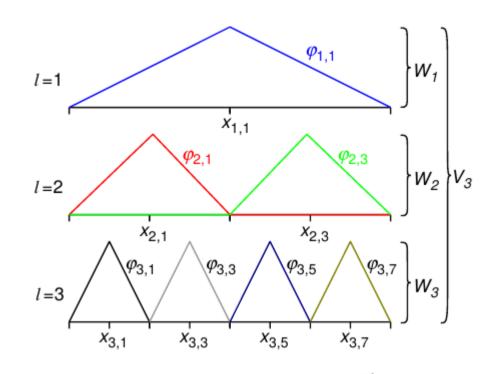


Fig.: 1-d basis functions  $\phi_{l,i}$  and the corresponding grid points up level l=3 in the hierarchical basis.

**Note:** supports of all basis functions of W<sub>k</sub> mutually disjoint!

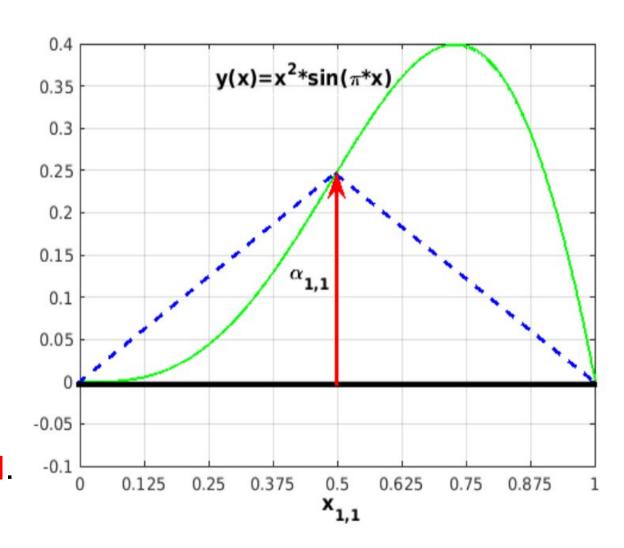
### Piecewise Linear Interpolation: Level I

# Coefficients: hierarchical surpluses

They correct the interpolant of level l-1 at  $\vec{x}_{l,i}$  to the actual value of  $f(\vec{x}_{l,i})$ 

#### **Nested structure:**

Evaluate function only at points that are unique to the new level.



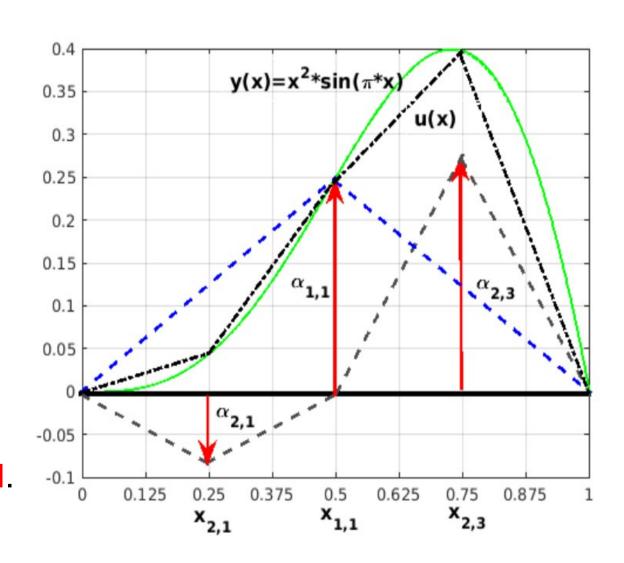
### Piecewise Linear Interpolation: Level II

# Coefficients: hierarchical surpluses

They correct the interpolant of level l-1 at  $\vec{x}_{l,i}$  to the actual value of  $f(\vec{x}_{l,i})$ 

#### **Nested structure:**

Evaluate function only at points that are unique to the new level.



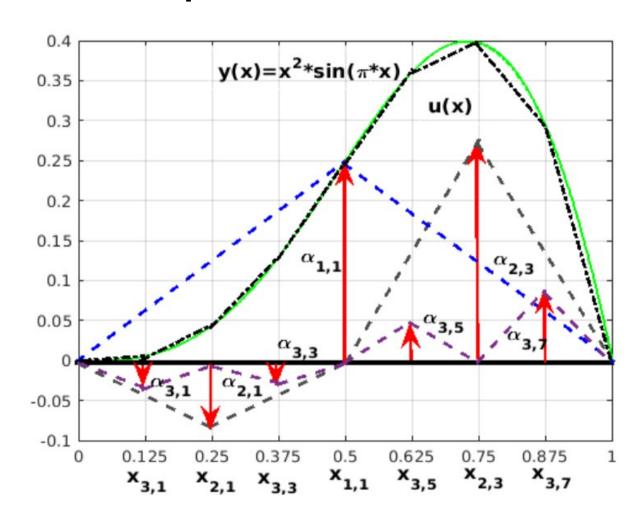
### Piecewise Linear Interpolation: Level III

# Coefficients: hierarchical surpluses

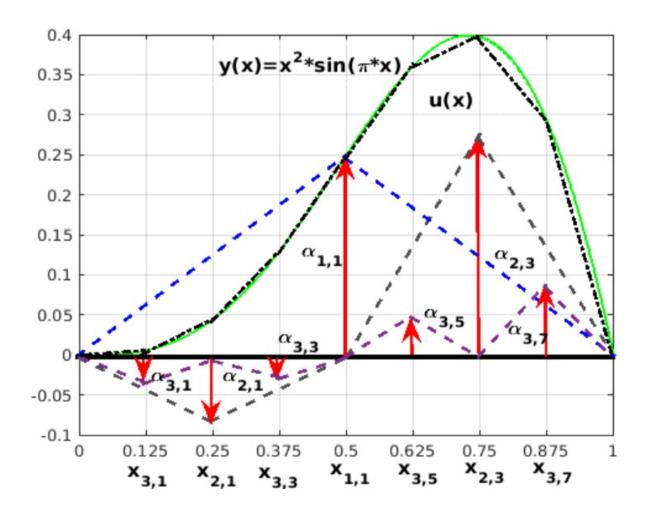
They correct the interpolant of level l-1 at  $\vec{x}_{l,i}$  to the actual value of  $f(\vec{x}_{l,i})$ 

#### **Nested structure:**

Evaluate function only at points that are unique to the new level.



# **MOVIE**



### Non-zero Boundary Conditions

Want to be able to handle non-zero boundaries:

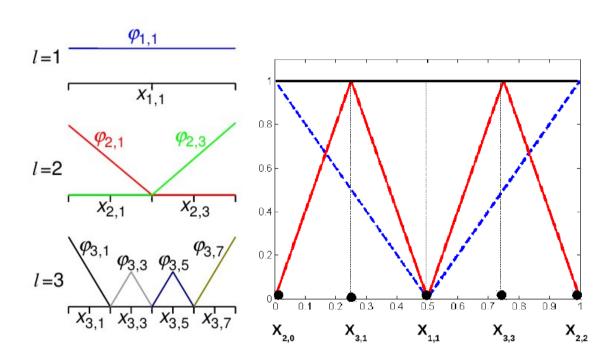
$$f|_{\partial\Omega} \neq 0$$

If we add naively points at boundaries, **3**<sup>d</sup> support nodes will be added.

Numerically cheapest way:

Modify basis functions and interpolate towards boundary.

Various choices possible!



**Fig.**: Example of modified 1d-basis functions According to Pflüger (2010), which are extrapolating towards the boundary (**left**). They are constant on level 1 and "**folded-up**" if adjacent to the boundary on all other levels. **Right**: "Modified" hat basis.

## Some definitions & notation

(see, e.g. Zenger (1991), Bungartz & Griebel (2004), Garcke (2012), Pflüger (2010),...)

- We will focus on the domain  $\Omega = [0,1]^d$  d: dimensionality; other domains: rescale
- introduce multi-indices:

grid refinement level: 
$$\vec{l} = (l_1, ..., l_d) \in \mathbb{N}^d$$

spatial position: 
$$\vec{i} = (i_1,...,i_d) \in \mathbb{N}^d$$

- Discrete, (Cartesian) full grid  $\,\Omega_{ec{l}}\,$  on  $\,\Omega$
- Grid  $\Omega_{\vec{l}}$  consists of points:  $\vec{x}_{\vec{l},\vec{i}} := (x_{l_1,i_1},...,x_{l_d,i_d})$

Where 
$$x_{l_t,i_t} := i_t \cdot h_{l_t} = i_t \cdot 2^{-l_t}$$
 and  $i_t \in \{0,1,...,2^{l_t}\}$ 

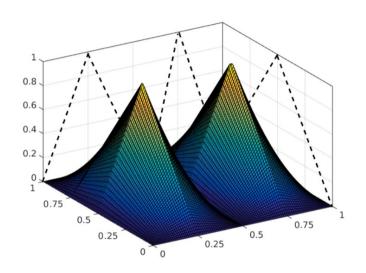
# Multi-Dimensional Interpolant

#### Extension to multi-d by a tensor-product construction:

Multi-d basis: 
$$\phi_{\vec{l},\vec{i}}(\vec{x}) := \prod_{t=1}^{d} \phi_{l_t,i_t}(x_t)$$

Index set: 
$$I_{\vec{l}} := \{\vec{i} : 1 \le i_t \le 2^{l_t} - 1, i_t \text{ odd}, 1 \le t \le d\}$$

Hierarchical increments: 
$$W_{\vec{l}} := \operatorname{span}\{\phi_{\vec{l},\vec{i}} : \vec{i} \in I_{\vec{l}}\}$$



#### Multi-d interpolant:

$$f(\vec{x}) \approx u(\vec{x}) = \sum_{|l|_{\infty} \le n} \sum_{\vec{i} \in I_{\vec{r}}} \alpha_{\vec{l}, \vec{i}} \cdot \phi_{\vec{l}, \vec{i}}(\vec{x})$$

Fig.: Basis functions of the subspace W<sub>2.1</sub>

# Why reality bites...

Interpolant consists of  $O(2^{nd})$  grid points

For sufficiently smooth f and its interpolant u, we obtain an asymptotic error decay of  $||f(\vec{x}) - u(\vec{x})||_{L_2} \in \mathcal{O}\left(h_n^2\right)$ 

But at the cost of

$$\mathcal{O}\left(h_n^{-d}\right) = \mathcal{O}\left(2^{nd}\right)$$

function evaluations → "curse of dimensionality"

Hard to handle more than 4 dimensions numerically

 $\rightarrow$  e.g. d=10, n = 4, 15 points/d, **5.8** x **10**<sup>11</sup> grid points

### 'Breaking' the curse of dimensionality I

Question: "can we construct discrete approximation spaces that are better in the sense that the same number of invested grid points leads to a higher order of accuracy?" YES √

(see, e.g. Bungartz & Griebel (2004))

→ If second mixed derivatives are bounded, then the hierarchical surpluses decay rapidly with increasing approximation level.

$$|\alpha_{\vec{l},\vec{i}}| = \mathcal{O}\left(2^{-2|\vec{l}|_1}\right)$$

### <u>`Breaking' the curse of dimensionality II</u>

(see, e.g. Bungartz & Griebel (2004)

Strategy of constructing sparse grid: leave out those subspaces from full grid that only contribute little to the overall interpolant.

Optimization w.r.t. number of degrees of freedom (grid points) and the approximation accuracy leads to the sparse grid space of level *n*.

$$V_{0,n}^S := \bigoplus_{|\vec{l}|_1 \le n+d-1} W_{\vec{l}}$$

Interpolant: 
$$f_{0,n}^S(\vec{x}) \approx u(\vec{x}) = \sum_{|l|_1 \leq n+d-1} \sum_{\vec{i} \in I_{\vec{l}}} \alpha_{\vec{l},\vec{i}} \cdot \phi_{\vec{l},\vec{i}}(\vec{x})$$

$$\text{\# grid points:} \, \mathcal{O}\left(h_n^{-1} \cdot \left(\log(h_n^{-1})\right)^{d-1}\right) = \, \mathcal{O}\left(2^n \cdot n^{d-1}\right) << \, \mathcal{O}\left(h_n^{-d}\right) = \mathcal{O}\left(2^{nd}\right)$$

Accuracy of the interpolant:  $\mathcal{O}\left(h_n^2 \cdot \log(h_n^{-1})^{d-1}\right)$  vs.  $\mathcal{O}\left(h_n^2\right)$ 

# Sparse grid construction in 2D

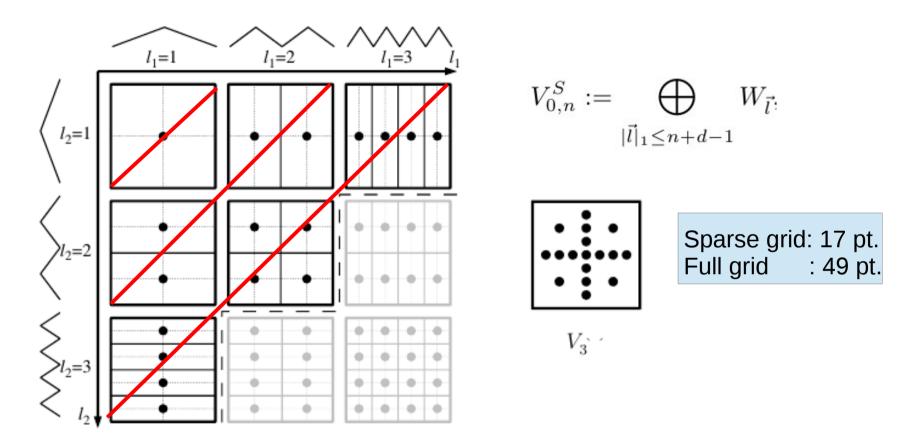
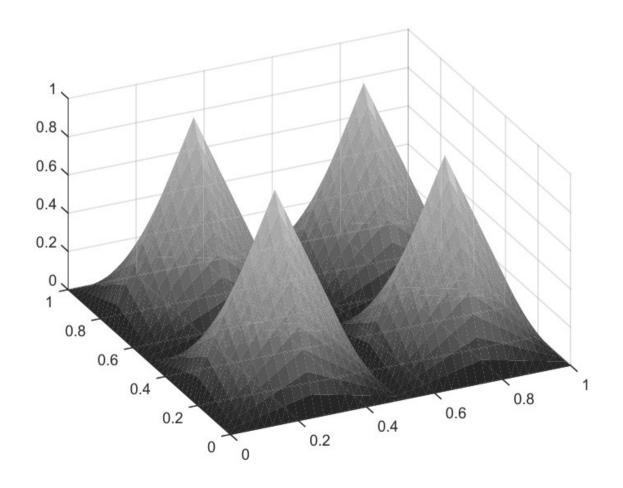


Fig.: Two-dimensional subspaces  $W_1$  up to I=3 ( $h_3=1/8$ ) in each dimension.

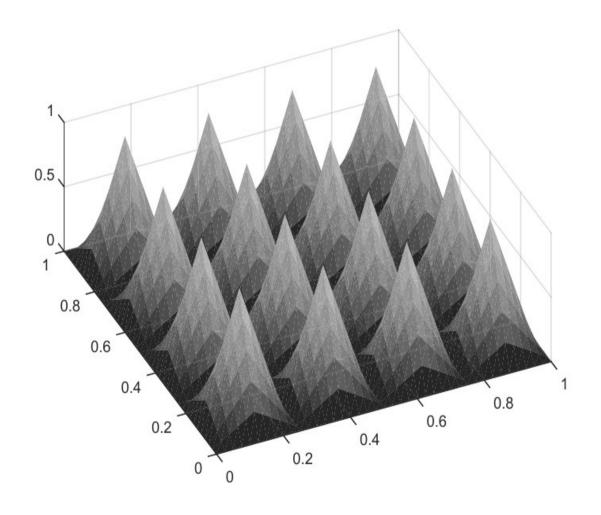
The optimal a priori selection of subspaces in shown in black (left) and the Corresponding sparse grid of level n = 3 (right).

For the full grid, the gray subspaces have to be used as well.

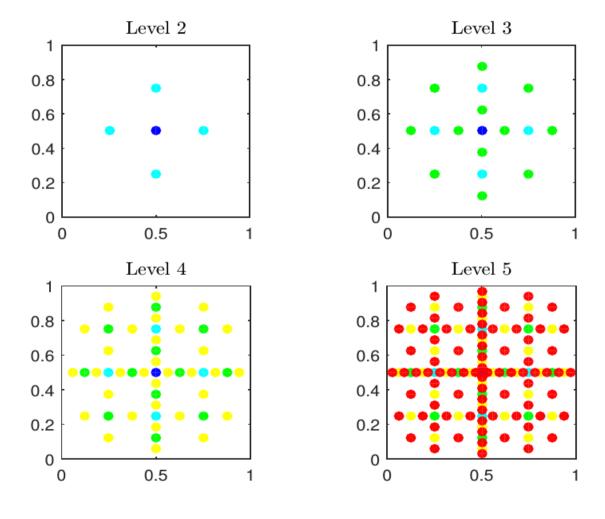
# Basis Functions of $W_{2,2}$ — Included in $V_3$



# Basis Functions of $W_{3,3}$ — not Included in $V_3$



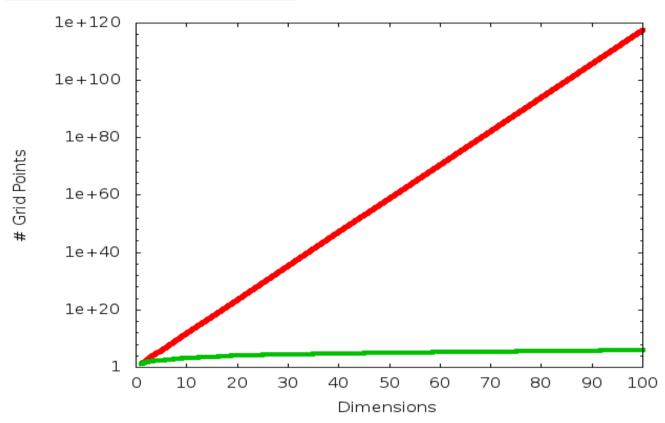
# Sparse Grid of Increasing level



II. From full grids to sparse grids

### **Grid Points**

d	$ V_n $	$ V_{0,n}^{S} $
1	15	15
2	225	49
3	3375	111
4	50'625	209
5	759'375	351
10	$5.77 \cdot 10^{11}$	2'001
15	$4.37 \cdot 10^{17}$	5'951
20	$3.33 \cdot 10^{23}$	13'201
30	$1.92 \cdot 10^{35}$	41'601
40	$1.11 \cdot 10^{47}$	95'201
50	$6.38 \cdot 10^{58}$	182'001
100	>Googol	1'394'001



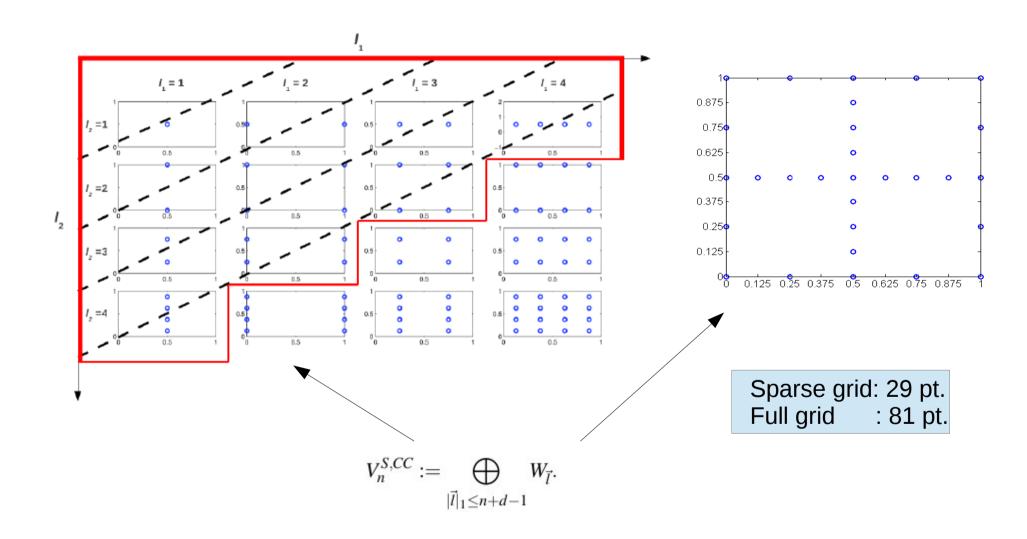
**Tab.**: Number of grid points for several types of sparse grids of level n = 4.

Middle: Full grid; right: classical sparse grid with no points at the boundaries.

Fig.: Number of grid points growing with dimension (full grid vs. sparse grid).

## Sparse Grid with non-zero boundaries

(see, e.g. Bungartz & Griebel (2004))



### **Hierarchical Integration**

High-dimensional integration easy with sparse grids, e.g. compute expectations Let's assume uniform probability density:

$$\mathbb{E}\left[u(\vec{x})\right] = \sum_{|l|_1 \le n + d - 1} \sum_{\vec{i} \in I_{\vec{l}}} \alpha_{\vec{l}, \vec{i}} \int_{\Omega} \phi_{\vec{l}, \vec{i}}(\vec{x}) d\vec{x}$$

The one-dimensional integral can now be computed analytically (Ma & Zabras (2008))

$$\int_{0}^{1} \phi_{l,i}(x) dx = \begin{cases} 1, & \text{if } l = 1\\ \frac{1}{4} & \text{if } l = 2\\ 2^{1-l} & \text{else} \end{cases}$$

Note that this result is independent of the location of the interpolant to dilation And translation properties of the hierarchical basis functions.

→ Multi-d integrals are therefore again products of 1-d integrals.

We denote 
$$\int_{\Omega}\phi_{l,i}\left(\vec{x}\right)d\vec{x}=J_{\vec{l},\vec{i}}$$
 
$$\longrightarrow \mathbb{E}\left[u(\vec{x})\right]=\sum_{|l|_{1}\leq n+d-1}\sum_{\vec{i}\in I_{\vec{l}}}\alpha_{\vec{l},\vec{i}}\cdot J_{\vec{l},\vec{i}}$$

# Where are Sparse Grids used?

For a review, see, e.g. Bungartz & Griebel (2004)

Sparse grid methods date back to Smolyak(1963)

**BUT: Smolyak used global polynomials!** 

So far, methods applied to:

-High-dimensional integration

e.g. Gerstner & Griebel (1998), Bungartz et al. (2003),...

-Interpolation

e.g. Barthelmann et al. (2000), Klimke & Wohlmut (2005),...

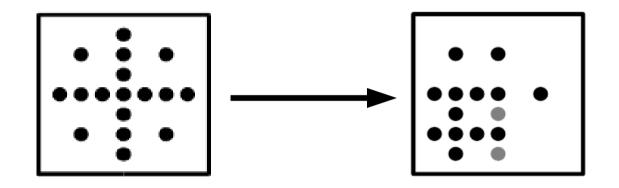
-Solution of PDEs

e.g. Zenger (1991), Griebel (1998),...

More fields of application: regressions, data mining, likelihood estimations, option pricing, data compression, dynamic economic models...

e.g. Kubler & Kruger (2004), Winschel & Kraetzig (2010), Judd et al. (2013) → Smolyak; global basis functions.

## **III. Adaptive Sparse Grids**

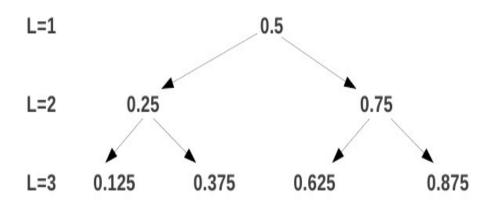


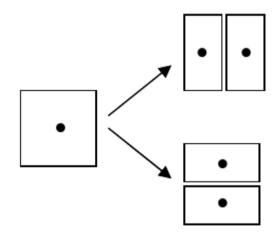
## Sketch of adaptive refinement

See, e.g. Ma & Zabaras (2008), Pflüger (2010), Bungartz (2003),...

- -Surpluses should quickly decay to zero
- -Use hierarchical surplus as error indicator.
- -Automatically detect
  "discontinuity regions" and
  adaptively refine the points in this
  region.
- -Each grid point has **2d** neighbours
- -Add neighbour points, i.e. locally refine interpolation level from *I* to *I*+1

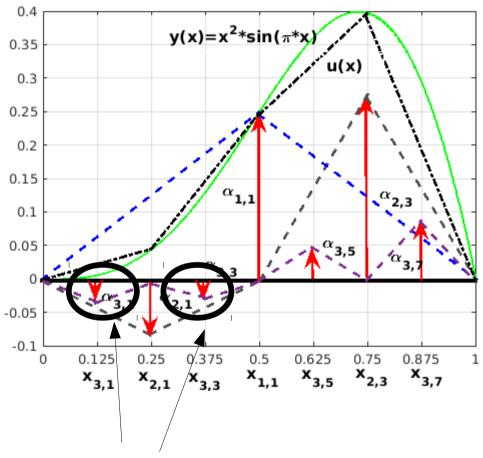
-Criterion: **e.g.**  $|\alpha_{\vec{l},\vec{i}}| \geq \epsilon$ 





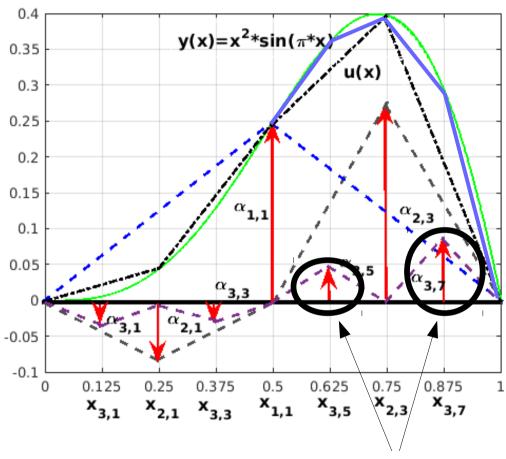
**top panel:** tree-like structure of sparse grid. **lower panel:** locally refined sparse grid in 2D.

## Example I



Small – below threshold

## Example II



Add points – above threshold

#### Test in 1d

(See Genz (1984) for test functions)

#### Test function:

$$f(x) = \frac{1}{|0.5 - x^4| + 0.01}$$

Error both for full grid and adapt. sparse grid of  $O(10^{-2})$ .

#### Error measure:

→ 1000 random points from [0,1]

$$e = \max_{i=1,\dots,1000} |f\left(\vec{x_i}\right) - u\left(\vec{x_i}\right)|$$

Full grid: 1023 points

Adaptive sparse grid: 109 points.

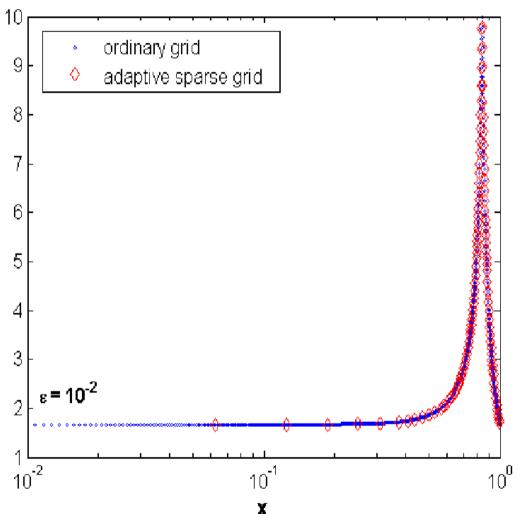


Fig.: Blue: Full grid; red: adaptive sparse grid.

#### Test in 2d

Test function:

$$\frac{1}{|0.5 - x^4 - y^4| + 0.1}$$

Error:

 $O(10^{-2})$ 

Full grid:

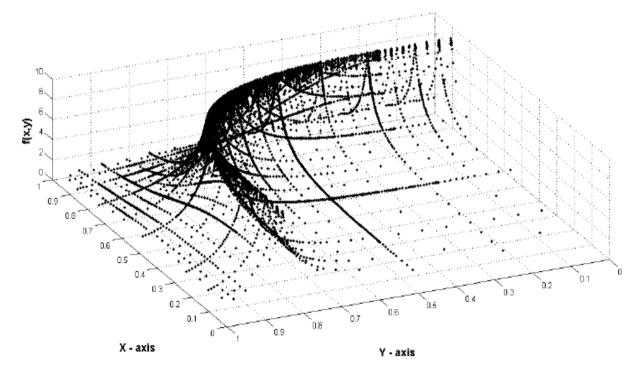
 $\rightarrow$   $O(10^9)$  points

Sparse grid:

→ **311,297** points

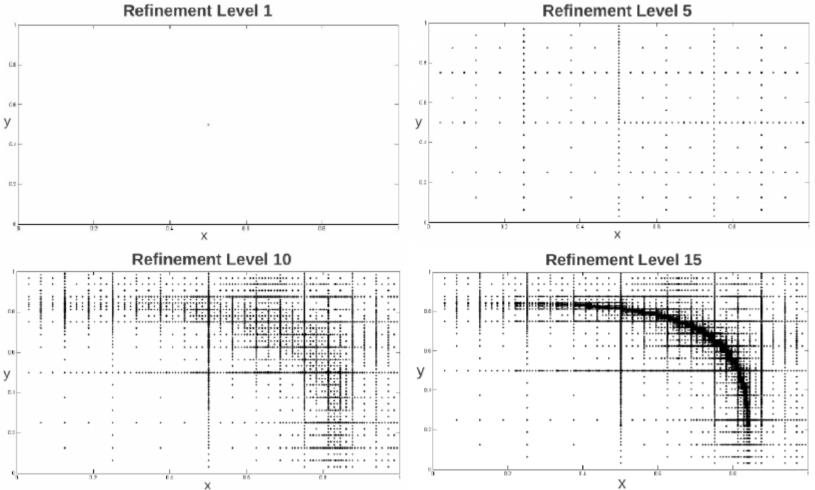
Adaptive sparse grid:

**→ 4,411 points** 



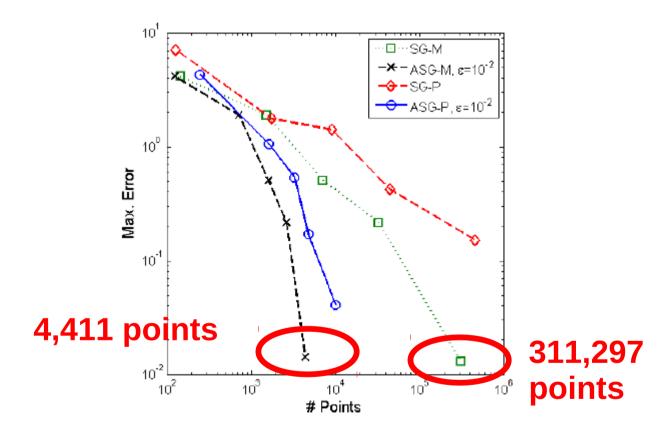
**Fig.**: 2d test function and its corresponding grid points after 15 refinement steps.

#### **Movie**



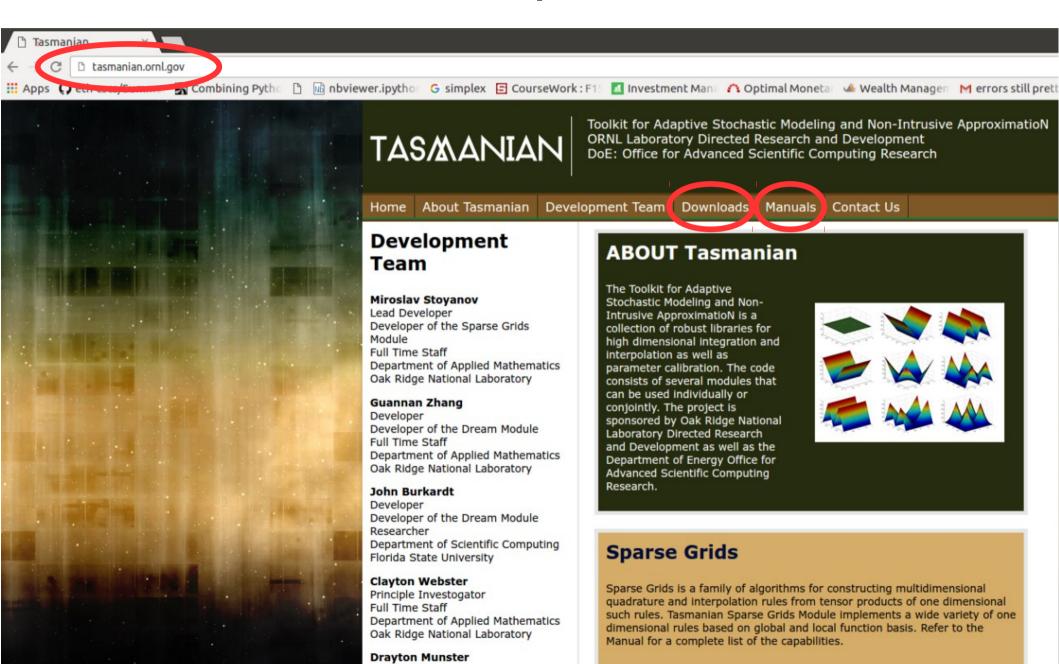
**Fig.**: Evolution of the adaptive sparse grid with a **threshold for refinement of 10^{-2}**. The refinement levels displayed are L = 1, 5, 10, 15.

## Convergence



**Fig.**: Comparison of the interpolation error for **conventional and adaptive sparse grid interpolation** (two different adaptive sparse grid choices).

## <u>TASMANIAN</u> – open source ASG



#### Software tutorial in the afternoon!!

The Toolkit for Adaptive Stochastic Modeling and Non-Intrusive ApproximatioN http://tasmanian.ornl.gov/

TASMANIAN Sparse Grids v3.1 (February 2016).

Very recent open source library written in CPP:

- → Contains "ordinary and adaptive" sparse grids.
- → Many more basis functions (global polynomials, wavelets,...).
- → Interfaces to Python and Matlab.
- → Moderately parallelized (with OpenMP).

## Compile & run TASMANIAN\*

!!! READ THE \*\*\* MANUAL (RTFM) - p.50ff !!!

#### 1. go to TASMANIAN:

> cd zice17/scheidegger/sparse grids/TasmanianSparseGrids

#### 2. compile:

> make

#### 3. go to simple example:

> cd zice17/scheidegger/sparse\_grids/TasmanianSparseGrids/ZICE17\_Matlab

#### 4. let's have a look at the example:

> tsg\_example\_ZICE17.m

#### 5. launch matlab & run example:

- > matlab -nojvm (no gui)
- > tsg\_example\_ZICE17()

#### 6. NOTE: Tasmanian [-1,1]^d instead of [0,1]^d

If you are interested in CPP code examples, TASMANIAN provides examples here:

- > cd Tzice17/scheidegger/sparse grids/TasmanianSparseGrids/Example/example.cpp
- > make

#### Exercises

Create sparse grids based on different analytical test functions, e.g. Genz (1984).

- $\rightarrow$  different test functions can be obtained by varying  $c = (c_1, \dots, c_d)$  (c>0) and  $w = (w_1, \dots, w_d)$
- → difficulty of functions is monotonically increasing with c.
- $\rightarrow$  randomly generate 1,000 test points and compute error(s):  $e = \max_{i=1,\dots,1000} |f(\vec{x_i}) u(\vec{x_i})|$ .
- → play with adaptive/non-adaptive sparse grids/refinement level and criterion.
- $\rightarrow$  generate convergence plots (number of points versus error as done above).

1. OSCILLATORY: 
$$f_1(x) = \cos\left(2\pi w_1 + \sum_{i=1}^d c_i x_i\right),$$

2. PRODUCT PEAK: 
$$f_2(x) = \prod_{i=1}^{d} (c_i^{-2} + (x_i - w_i)^2)^{-1}$$

1. OSCILLATORY: 
$$f_1(x) = \cos\left(2\pi w_1 + \sum_{i=1}^d c_i x_i\right),$$
  
2. PRODUCT PEAK:  $f_2(x) = \prod_{i=1}^d \left(c_i^{-2} + (x_i - w_i)^2\right)^{-1},$   
3. CORNER PEAK:  $f_3(x) = \left(1 + \sum_{i=1}^d c_i x_i\right)^{-(d+1)},$ 

4. GAUSSIAN: 
$$f_4(x) = \exp\left(-\sum_{i=1}^{d} c_i^2 t (x_i - w_i)^2\right)$$

5. CONTINUOUS: 
$$f_5(x) = \exp\left(-\sum_{i=1}^d c_i |x_i - w_i|\right)$$

4. GAUSSIAN:  $f_4(x) = \exp\left(-\sum_{i=1}^{d} c_i^2 t(x_i - w_i)^2\right),$ 5. CONTINUOUS:  $f_5(x) = \exp\left(-\sum_{i=1}^{d} c_i |x_i - w_i|\right),$ 6. DISCONTINUOUS:  $f_6(x) = \begin{cases} 0, & \text{if } x_1 > w_1 \text{ or } x_2 > w_2, \\ \exp\left(\sum_{i=1}^{d} c_i x_i\right), & \text{otherwise.} \end{cases}$ 

January 31st, 2017

# 1. III. Putting things together: Iterative schemes\*, Adaptive Sparse Grids, HPC



#### IRBC with Adjustment Costs and Irreversible Investment

- Use test case from JEDC project on computational methods (Den Haan et al. 2011, Juillard and Villemot 2011, Kollmann et al. 2011)
- N countries facing productivity shocks and capital adjustment costs
  - $\Rightarrow$  countries differ in productivity, **a** (stochastic and exogen.), and capital stock, **k** (endogen.)
  - $\Rightarrow$  dimension of the state space is 2N
  - ⇒ recursive equilibrium is characterized by policy  $p:R_{+}^{2N} \Rightarrow R_{+}^{N+1}$  mapping state into N capital choices and 1 Lagrange multiplier (as markets are complete)
- Extension: Investment in each country is irreversible:
  - ⇒ recursive equilibrium is characterized by policy  $p:R_{+}^{2N} \Rightarrow R_{+}^{2N+1}$  mapping state into N capital choices, 1 Lagrange multiplier, and N Karush-Kuhn-Tucker multipliers

## Time Iteration Algorithm: Detail

$$g_{t+1}^j := k_{t+1}^j/k_t^j - 1, \ g_{t+2}^j := k_{t+2}^j/k_{t+1}^j - 1,$$

$$\forall j : \mathbf{\lambda}_t \cdot \left[1 + \phi \cdot g_{t+1}^j\right] - \beta \cdot \mathbb{E}_t \left\{ \mathbf{\lambda}_{t+1} \cdot \left[a_{t+1}^j \cdot A \cdot \alpha \cdot (k_{t+1}^j)^{\alpha - 1} + (1 - \delta) + \frac{\phi}{2} \cdot g_{t+2}^j \cdot \left(g_{t+2}^j + 2\right)\right] \right\} = 0,$$

$$\sum_{j=1}^N \left(a_t^j \cdot A \cdot (k_t^j)^{\alpha} + k_t^j \cdot \left((1 - \delta) - \frac{\phi}{2} \cdot (g_{t+1}^j)^2\right) - k_{t+1}^j - \left(\frac{\mathbf{\lambda}_t}{\tau_j}\right)^{-\gamma^j}\right) = 0.$$

$$\mathbf{1} \text{ aggregate resource constraint}$$

We solve the model by iterating on these FOCs, i.e. at each grid point

$$\left(a_t^1,\ldots,a_t^N,k_t^1,\ldots,k_t^N\right)$$
 - Current grid points

solve for the unknown policy variables

$$(k_{t+1}^1, \dots, k_{t+1}^N, \lambda_t)$$
 Solution of system of Eqs. At the current iteration

given the known policy functions from last iteration

$$(k_{t+2}^1(a_{t+1}, k_{t+1}), \dots, k_{t+2}^N(a_{t+1}, k_{t+1}), \lambda_{t+1}(a_{t+1}, k_{t+1}))$$
  $\longrightarrow$  Interpolant

evaluated at next periods state

$$(a_t^1, \dots, a_t^N, k_t^1, \dots, k_t^N)$$
, where  $a_{t+1}^j = (a_t^j)^\rho \cdot e^{\sigma(e_t + e_t^j)}$ .

## Time Iteration Algorithm

Algorithm 1 Overview of the crucial steps of the time-iteration algorithm.

#### Time-Iteration Algorithm:

- 1. Make an initial guess  $p_{init}$  for next period's policy function. Set  $p_{next} = p_{init}$ . Choose an approximation accuracy  $\bar{\eta}$ .
- 2. Make one time-iteration step:
  - (a) Choose a maximal refinement level  $L_{max}$  and a fixed grid level  $L_0 \le L_{max}$ . Set l = 1, set  $G \subset X$  to be the level 1 grid on X, and set  $G_{old} = \emptyset$ .
  - (b) For each  $g \in G \setminus G_{old}$  compute the optimal policies p(g) by solving the system of equilibrium conditions

$$0 = \mathbb{E}\left\{f\left(g, x_{t+1}, p\left(g\right), p_{next}\left(x_{t+1}\right)\right) | g, p(g)\right\},\$$
$$x_{t+1} \sim F\left(\cdot | g, p(g)\right),\$$

given next period's policy  $p_{next}$ . Construct the hierarchical surpluses of level l.

(c) Generate  $G_{new}$  from G by adding for each  $g \in G_l \setminus G_{old}$  its 2d neighbouring points, if either  $l < L_0$  or

$$||p(g) - \tilde{p}(g)||_{\infty} > \varepsilon$$

where the policy  $\tilde{p}(g)$  is given by interpolating between  $\{p(g)\}_{g \in G_{old}}$ . Note that if  $G_{old}$  is of level 2, then each point does not have 2d but only d neighbouring points (cf. Fig. 3.4).

- (d) If  $G_{new} = G$  or  $l = L_{max}$ , then set  $G = G_{new}$  and go to (e), else set  $G = G_{new}$ , l = l + 1 and go to (b).
- (e) Define the policy function p as the sparse grid interpolation of  $\{p(g)\}_{g\in G}$ .
- (f) Calculate (an approximation for) the error, e.g.

$$\eta = \|p - p_{next}\|_{\infty}.$$

If  $\eta > \bar{\eta}$ , set  $p_{next} = p$  and go to (a), else go to step 3.

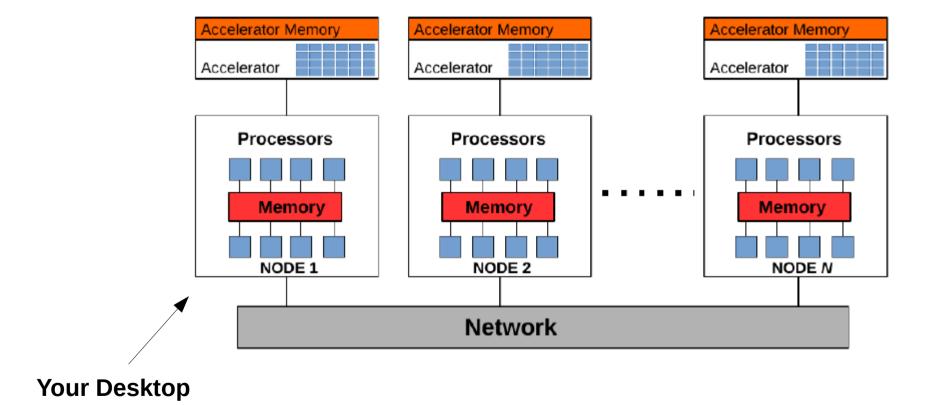
3. The (approximate) equilibrium policy function is given by p.

# "To pull a bigger wagon, it is easier to add more oxen than to grow a gigantic ox" (Skjellum et al. 1999)

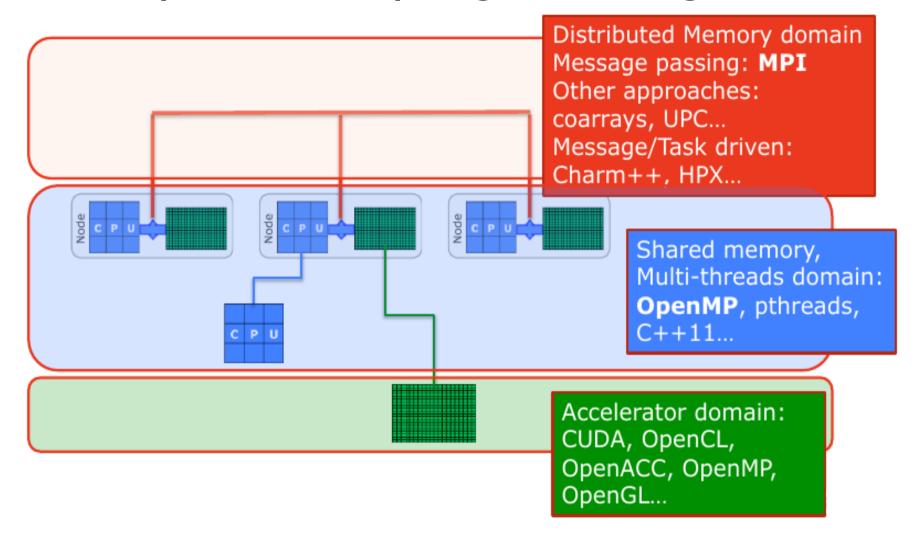


Piz Daint (Swiss Supercomputing Centre); 10x 10<sup>15</sup> Flops/Sec. = 1500y of a laptop in a day.

## Today's HPC systems



#### Overall picture of programming models



→ Creating `good' HPC software can be very difficult...

## Speedup, Efficiency & Amdahl's Law

T(p,N) := time to solve problem of total size N on p processors.

**Parallel speedup**: S(p,N) = T(1,N)/T(p,N)

→ Compute same problem with more processors in **shorter time**.

**Parallel Efficiency:** E(p,N) = S(p,N)/p

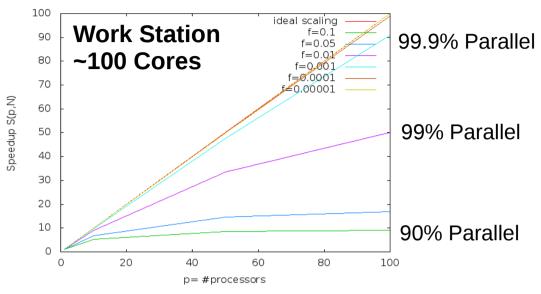
Amdahl's Law: T(p,N) = f \* T(1,N) + (1-f) T(1,N)/p

f...sequential part of the code that can not be done in parallel

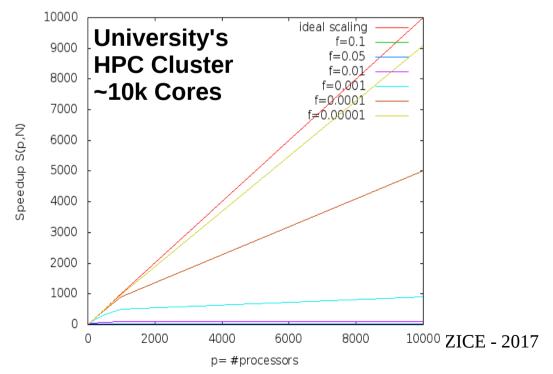
$$S(p,N) = T(1,N)/T(p,N) = 1 / (f + (1-f)/p)$$

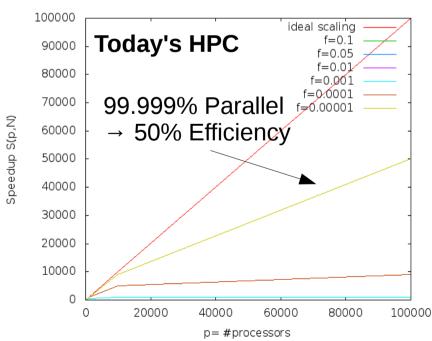
For p  $\rightarrow$  infinity, speedup is limited by S(p,N) < 1/f

## <u>Amdahl's Law: Scaling is tough</u>



For  $p \rightarrow infinity$ : Speedup is limited by S(p,N) < 1/f





## Parallel time iteration/DP algorithm

-Our implementation:

#### **Hybrid parallel**

(MPI & Intel TBB & GPU (CUDA/THRUST)).

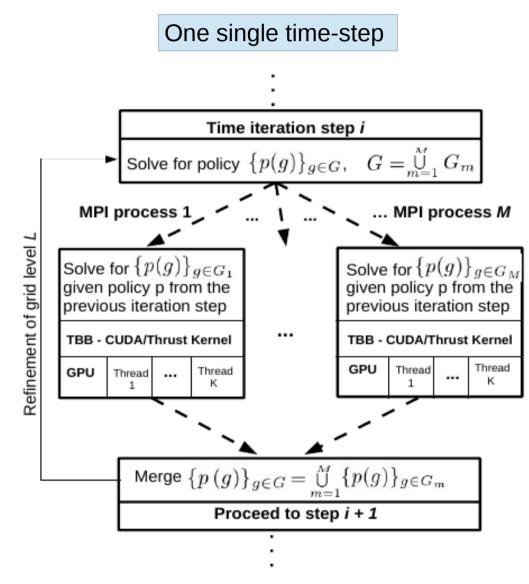
-newly generated points are distributed via MPI

#### Solve optimizations/ nonlinear equations locally

(e.g. IPOPT (Waechter & Biegler (2006)).

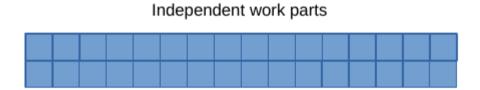
In parallel: `messy'!

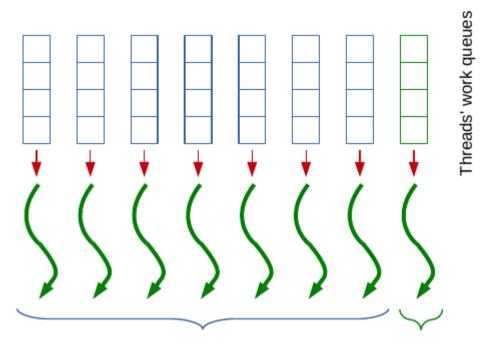
- → policy from previous iteration visible on all MPI processes.
- → we have to ensure some sort of `load balancing'.



#### Intel® Threading Building Blocks (TBB)

-TBB maps different threads, similar to OpenMP.

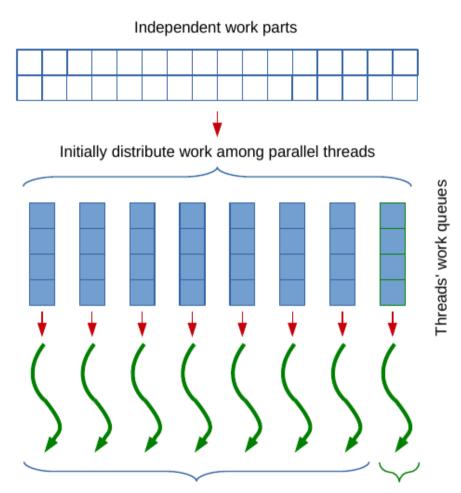




Threads mapped to CPU cores Thread mapped to GPU

#### Intel® Threading Building Blocks (TBB)

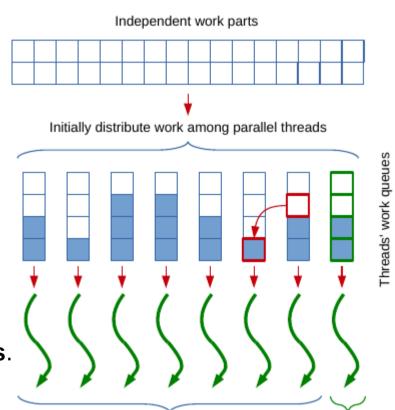
- -TBB maps different threads, similar to OpenMP.
- -Every thread is initially assigned an equal logical queue of tasks.



Threads mapped to CPU cores Thread mapped to GPU

#### Intel® Threading Building Blocks (TBB)

- -TBB maps different threads, similar to OpenMP.
- -Every thread is initially assigned an equal logical queue of tasks.
- -However, different tasks may be processed faster or slower, due to differences between tasks and/or compute cores
- -TBB approach to work balancing: once one thread runs out of tasks, "steal" a task from another thread, which makes slower progress.
- -We map one extra thread onto **GPU**
- → CPU cores and GPU process interpolation tasks together.

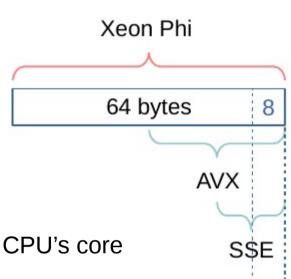


Threads mapped to CPU cores Thread mapped to GPU

#### **AVX** vectorization

Brumm, Mikushin, Scheidegger, Schenk (2014 – submitted)

-All modern CPUs have vector registers to process from 16 (SSE – old CPUs) to 64 (Xeon Phi) bytes of data simultaneously.



scalar

double

- 2012 and newer CPU can process 4 doubles with one instruction (AVX Advanced Vector Extensions)
- Running code without vectorization use of only 1/4 of CPU's core compute power (e.g. Piz Daint's CPUs)
- Compilers try to vectorize scalar code automatically, but usually succeed in simple cases only.
- → we need to develop vector-aware code, in order to make it efficient!

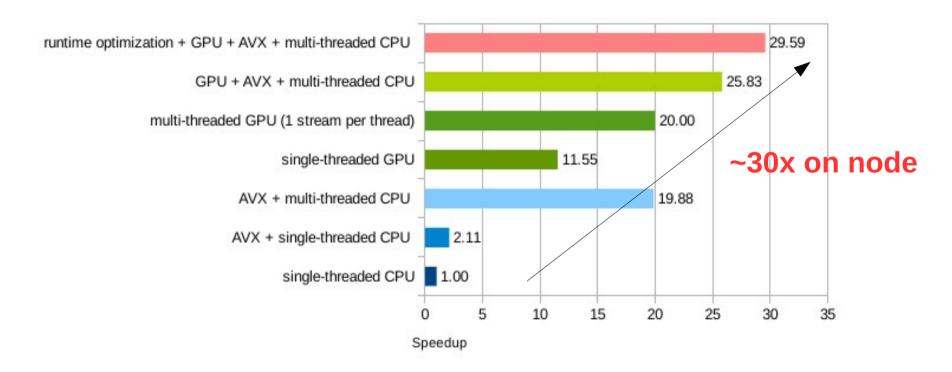
Example of scalar loop and its vectorized equivalent:

```
for (int i = 0; i < N; i++) y[i] += alpha * x[i];</pre>
```

```
for (int i = 0; i < N / 8; i++)
    _mm512_store_pd((void *)(y[8*i]), _mm512_add_pd( _mm512_load_pd((void *)(y[8*i])),
    _mm512_mul_pd(_mm512_set1_pd(alpha), _mm512_load_pd((void *)(x[8*i]))) ));</pre>
```

## Single-node Code Optimization

Brumm, Mikushin, Scheidegger, Schenk (2015)

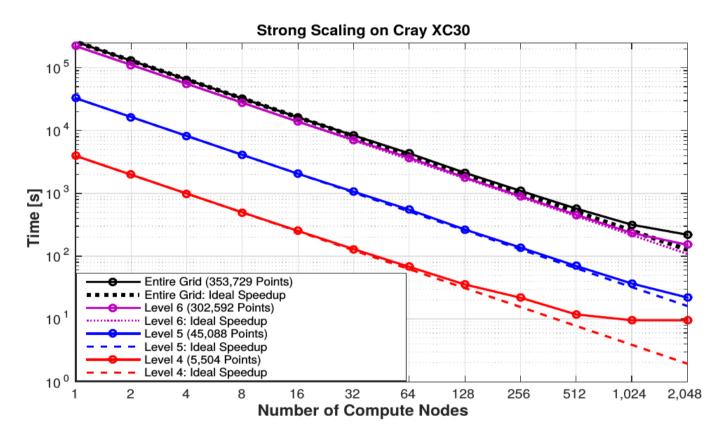


#### Notes:

- Level 2 (of an IRBC with binding constraints 128 grid points)
- Fully optimized code on 1 core (bitwise shifts, code inline, replace divisions where possible,...)
- 1 node today consists of several cores plus often a GPU (Piz Daint: Kepler K20X).
- AVX: Vectorization for 2012+ processors ("advanced vector extension")

#### A Strong Scaling Example

nodes are equipped with an 8-core 64-bit Intel SandyBridge CPU (Intel® Xeon® E5-2670), an NVIDIA® Tesla® K20X



**Fig**.: strong scaling of the code.

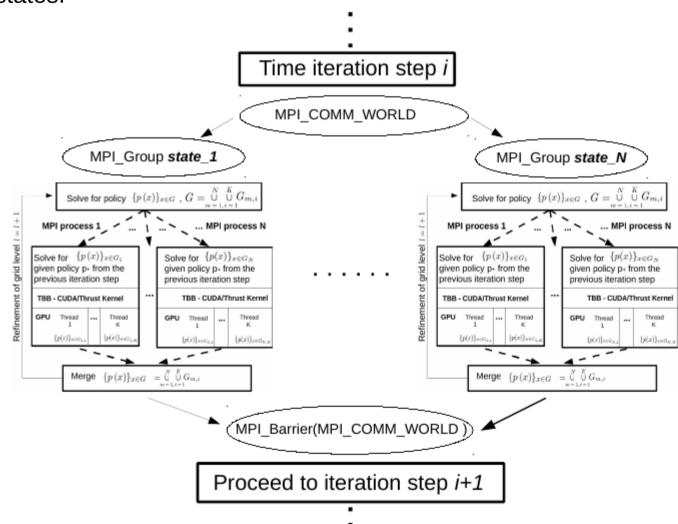
Problem: one timestep of an 16d IRBC, fixed refinement level 5.

Overall speedup more than  $\bf 3$  orders of magnitude (cf. 1 single node) .

## Going beyond IRBC → OLG

Brumm, Kübler, Scheidegger (2015)

- → OLG Model with 60 continuous state variables.
- → 4 discrete states.

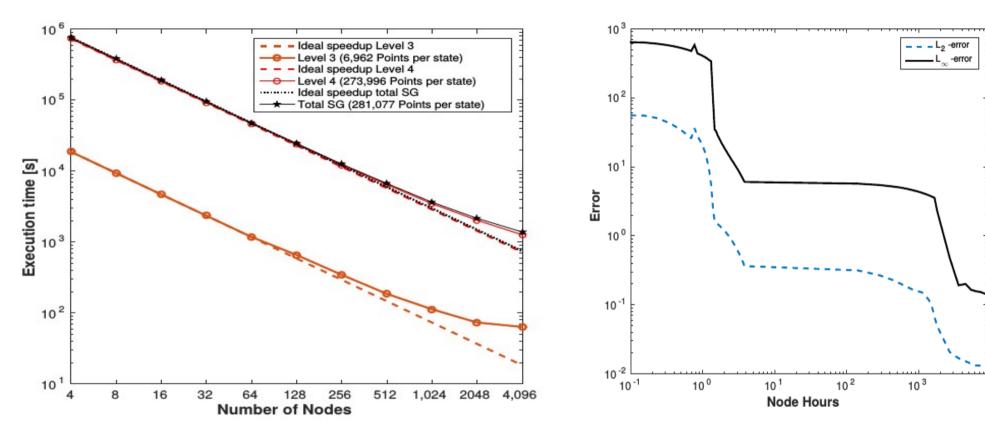


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#### <u>Discrete states: scaling & convergence</u>

Scheidegger et. al (2017) – in preparation (draft available at https://sites.google.com/site/simonscheidegger/publications)



- → scales ~linearly with number of discrete states, since they are fully independent.
- → Can use 80% of system with ~60% efficiency (this model).
- → Prepare code for exa-scale systems (Xeon Phi Knight landing).

#### Results for Smooth IRBC Model

Non-adaptive sparse grid of fixed level produces stable accuracy when dimension is increased massively:

Dimension	Level	Points	Max. Error	Avg. Error
4	3	41	-2.95	-3.18
12	3	313	-2.81	-3.27
20	3	841	-2.93	-3.30
50	3	5,101	-2.64	-3.33
100	3	20,201	-2.79	-3.33
4	4	137	-3.04	-3.65
12	4	2,649	-3.04	-3.83
20	4	11,561	-3.00	-3.73

All errors are given in log 10 -scale.

## Results for Non-Smooth IRBC Model: Finer Grids

Non-adaptive sparse grid has problems with non-smooth model:

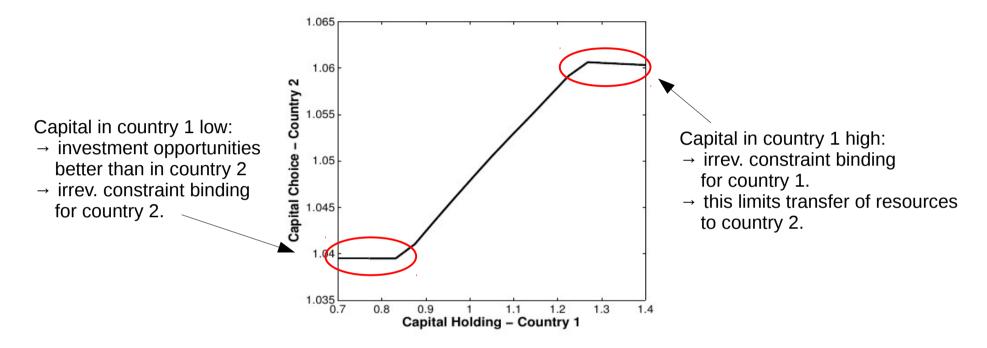
Dimension	Level	Points	Max. Error	Avg. Error
4	5	401	-2.11	-2.93
4	7	2,929	-2.32	-3.12
4	9	18,945	-2.45	-3.32

Adaptive sparse grid can overcome problems with non-smooth model → they provide higher accuracy with less points:

$\epsilon$	Max. Level Reached	Points	Max. Error	Avg. Error
0.01	7 (2,929)	245	-2.23	-2.88
0.005	9 (1,945)	559	-2.42	-2.98
0.0025	13 (643,073)	2,346	-2.68	-3.32
0.001	14 (3,502,081)	14,226	-2.91	-3.73

All errors are given in log 10 -scale.

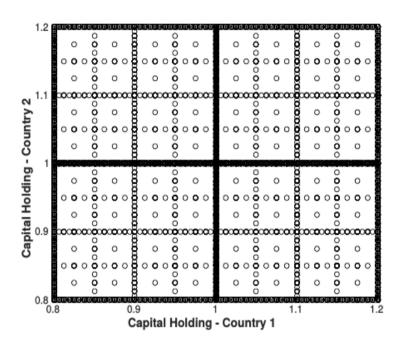
#### IRBC with irreversible investment

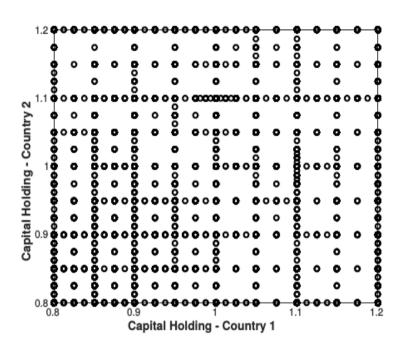


**Fig.**: Capital choice of country 2 as a function of capital holding of country 1. All other state variables of this model are kept fixed at steady state (2N = 4d). The 4-d policy function was interpolated on an adaptive sparse grid ( $\epsilon$  = 0.0033).

Note: kink is (2N -1) - dimensional hypersurface in 2N - dim state space.

## IRBC with binding constraints





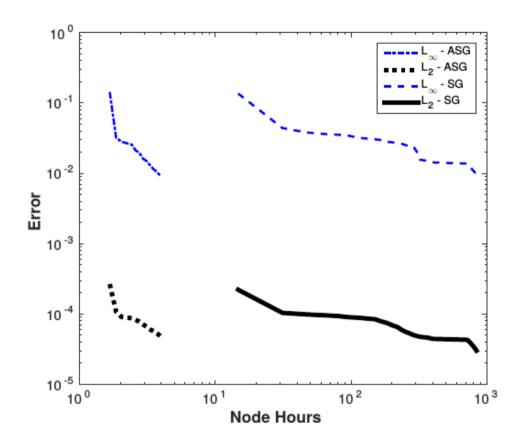
**Fig.**: 2-d projections of two different grids.

Left: `classical' sparse grid of level 9 (18,945 points),

**Right**: adaptive grid with refinement threshold  $\varepsilon = 0.001$  (14,226 points).

The x-axis shows capital holding of country 1, the y-axis shows capital holding of country 2, while the productivities of the two countries are kept fixed at their unconditional means.

# Models with binding constrains: massive speedup due to adaptivity



Dimension	Points	Max. Error	Avg. Error	$ V_8^{S,CC} $
4	245	-2.22	-2.88	18,945
6	684	-2.26	-2.73	127,105
8	931	-2.02	-2.66	609,025
10	2,790	-1.97	-2.54	2,148,960
12	4,239	-1.81	-2.48	7,451,394
16	8,569	-1.94	-2.36	52,789,761
20	9,098	-1.96	-2.35	$\gg 10^{8}$

**Tab.**: Comparison of a sparse and adapt. sparse grid of comparable accuracy.

**Fig.**: 8d model with binding constraints. model run with/without adaptive sparse grids. Relative error among two consecutive time-steps. 10k points drawn from uniform distribution.

#### **Summary**

 Method perfectly suited to solve high dimensional dynamic models with large amount of heterogeneity! (Method: Scalable & Flexible).

#### **Method very helpful to address:**

- High-dimensional, heterogeneous time-iteration & dynamic programming problems.
- International Real Business Cycle (IRBC) Models: Exchange Rates, Global Trade Imbalances.
- Dynamic Stochastic General Equilibrium (DSGE) Models: Monetary Policy, Business Cycle Fluctuations.
- Overlapping Generations (OLG) Models: Demographic Change, Social Security.
- · Option pricing.