Computer algebra models dynamics on a multigrid across multiple length and time scales

A. J. Roberts*

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Abstract

Methods for modelling dynamics posit just two time scales: a fast and a slow scale. But many applications, including many in continuum mechanics, possess a wide variety of space-time scales; often they possess a continuum of space-time scales. The computer algebra described here empowers an approach to modelling the dynamics of advection and diffusion with rigorous support for changing the resolved space-time scale by just a factor of two. The mapping of dynamics from a finer grid to a coarser grid may be iterated to generate a hierarchy of models across a wide range of space-time scales.

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*Computational Engineering and Sciences Research Centre, Dept Maths and Computing, University of Southern Queensland, Toowoomba, Queensland 4350, Australia.

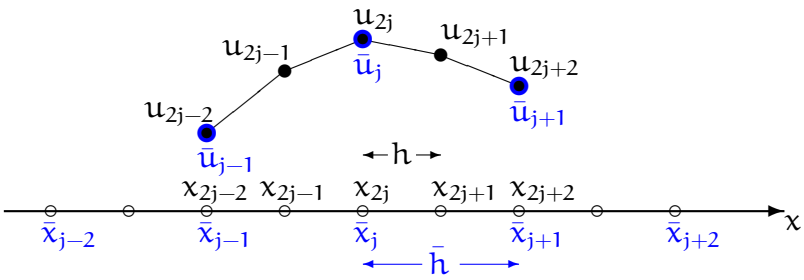

Figure 1: schematic picture of the equi-spaced fine grid, x_j, with spacing h, and grid values u_j. The coarse grid, $\bar{x}_j$, with spacing $\bar{h} = 2h$, and grid values $\bar{u}_j$ is superposed.

1 Introduction

Most multiscale mathematical methods for modelling disparate scales presume just two scales: small lengths and large lengths; fast times and long times; fast variations and slow variations; microscopic and macroscopic [3, 4, e.g.]. Most such methods then seek *effective* models or properties on the large/long/slow macroscales by 'averaging/homogenising over' the small/fast microscales [4, 6, 9, e.g.]. Here we implement in computer algebra a novel approach to modelling dynamics over the many length and time scales of a multigrid [1, e.g.]. Applications, results and relevance are detailed elsewhere [8].

Consider linear dynamics at any scale [8, §3.5]. Define a one dimensional grid x_j of constant spacing; at each grid point a grid value $u_j(t)$ evolves in time as shown in Figure 1. We transform the dynamics on this grid to dy-

namics on a grid of twice the spacing as also shown schematically in Figure 1. Introduce a, possibly artificial, 'ordering' parameter γ to decompose the fine grid dynamics as

$$\frac{du_j}{dt} = \left[\mathcal{L}_1 + \gamma\mathcal{L}_2 + \gamma^2\mathcal{L}_3 + \cdots + \gamma^{n-2}\mathcal{L}_{n-1}\right] u_j \,, \tag{1}$$

where the kth discrete operator $\mathcal{L}_k$ has stencil width $2k+1$; that is, $\mathcal{L}_k u_j$ only involves $u_{j-k}, \ldots, u_{j+k}$. This decomposition terminates, as written in (1), when we restrict attention, by working to errors $\mathcal{O}(\gamma^{n-1})$, to operators of some maximum finite width. Usually, not but necessarily, the 'ordering' parameter at one level in the grid hierarchy will be the coupling parameter in the dynamics at finer grid levels. Choose the ordering parameter so that evaluation at $\gamma = 1$ gives the physically relevant model, whereas $\gamma = 0$ provides a base for theory to support models at non-zero γ.

Divide the fine scale grid into overlapping coarse scale elements, notionally, by introducing $v_{j,i}(t) = u_{2j+i}$ for i parametrising the fine scale grid points within the jth element. Insisting on the operator $\mathcal{L}_1$ being conservative implies $\mathcal{L}_1$ represents advection-dispersion dynamics; thus the $\gamma = 0$ dynamics, $\dot{v}_{j,i} = \mathcal{L}_1 v_{j,i}$, then provide a sound base for centre manifold theory [8, §3.5]. As well as introducing the ordering parameter γ into the dynamics, introduce a parameter $\bar{\gamma}$ coupling neighbouring elements: couple neighbouring elements with the conditions

$$v_{j,\pm 2} = \bar{\gamma} v_{j\pm 1,0} + (1-\bar{\gamma}) v_{j,0} \,. \tag{2}$$

Defining $\bar{u}_j$ to measure the amplitude of the dynamics in the jth element, herein I choose $\bar{u}_j = u_{2j}$, centre manifold theory [2, 5] then supports a slow manifold, coarse grid, model [8, §2] of the dynamics (1) in the form

$$\frac{d\bar{u}_j}{dt} = \left[\bar{\gamma}\bar{\mathcal{L}}_1 + \bar{\gamma}^2\bar{\mathcal{L}}_2 + \bar{\gamma}^3\bar{\mathcal{L}}_3 + \cdots + \bar{\gamma}^{n-1}\bar{\mathcal{L}}_{n-1}\right] \bar{u}_j + \mathcal{O}\left(\bar{\gamma}^n, \gamma^{n-1}\right) , \tag{3}$$

for some coarse grid operators $\bar{\mathcal{L}}_k$ (implicitly a function of the ordering parameter γ) which will be of stencil width $2k+1$ as the parameter $\bar{\gamma}$ counts the number of interelement communications.

Renormalising the dynamics from the finer grid to the coarser grid requires two extra ingredients: remove the fine grid ordering parameter by setting $\gamma = 1$ (so operators $\bar{\mathcal{L}}_k$ are no longer a function of the ordering parameter γ); and introduce a coarse time scale $\bar{t} = t/\bar{\gamma}$ which is formally a long time scale for small $\bar{\gamma}$ but is the same time scale when evaluated for the physically relevant $\bar{\gamma} = 1$, then, upon dividing by $\bar{\gamma}$, the coarse grid dynamics become

$$\frac{d\bar{u}_j}{d\bar{t}} = \left[\bar{\mathcal{L}}_1 + \bar{\gamma}\bar{\mathcal{L}}_2 + \bar{\gamma}^2\bar{\mathcal{L}}_3 + \cdots + \bar{\gamma}^{n-2}\bar{\mathcal{L}}_{n-1}\right]\bar{u}_j + \mathcal{O}\left(\bar{\gamma}^{n-1}\right). \tag{4}$$

The coarse model (4) has exactly the same form as the fine model (1). By introducing a hierarchy of couplings (2), a hierarchy of times, which all collapse to the same real time when $\bar{\gamma} = 1$, and working to some order of error in interelement coupling, models of the form (1) are transformed and renormalised across the entire multigrid hierarchy.

2 Overview of the algorithm

Construct the slow manifold and the slow evolution thereon of discrete, linear, advection-dispersion equations across many levels of the hierarchy of a multigrid. Here we repeat the transformation across `maxlevel` grid levels to explore the renormalisation of the dynamics. At each level in the grid, an iteration constructs the appropriate slow manifold model.

```
                    ▷▷ rdoal ◁◁
% see camdmamlts.pdf for documentation
◁◁ doal preamble ▷▷
for level:=1:maxlevel do begin
  write theLevel:=level;
  ◁◁ doal initialise ▷▷
  ◁◁ doal iterate ▷▷
  ◁◁ doal fin ▷▷
  showtime;
```

```
end;
end;
```

3 Start with the preamble

Include the usual trivial formatting instructions.

```
                    ▷▷ doal preamble ◁◁
on div; off allfac; on revpri; on gcd;
factor gamb,gama;
linelength 70;
```

Choose various cases to analyse. First, possibly explore the relatively simple transformation from one level to the next of an isotropic conservative linear operator: it only involves even order operators. Note: `gama` denotes the 'small' ordering parameter γ of the evolution operator at the current level, whereas `gamb` denotes the coupling parameter $\bar{\gamma}$ of elements at the current level which in turn becomes the ordering parameter at the next coarser level. We always work to one higher order in $\bar{\gamma}$ than in γ because of the scaling of time at the coarser level by $\bar{\gamma}$.

```
                    ▷▷ doal preamble ◁◁+
if 0 then begin % simpler isotropic case
    c:=0;  d:=c1; cc:=0;
    let {gamb^5=>0,gama^4=>0};
    maxlevel:=1; end;
```

Second, possibly explore the hierarchy of models produced from a definite microscale system advection-dispersion system. Over nine levels it approaches upwind discretisations of advection on the macroscale.

```
                ▷▷ doal preamble ◁◁+
if 1 then begin % example advection diffusion
    c:=1;  d:=1; cc:=c2:=c3:=0;
    let {gamb^3=>0,gama^2=>0};
    maxlevel:=3; end;
```

Third, possibly explore the general transformation from one level to the next of general advection-dispersion.

```
                ▷▷ doal preamble ◁◁+
if 0 then begin % general advection-dispersion
    c:=-c11-gama*c21;  d:=c12+gama*c22;
    cc:=c23; c2:=c24; c3:=0;
    let {gamb^3=>0,gama^2=>0};
    maxlevel:=1; end;
```

Find the width of each element necessary for the width of the required slow manifold model.

```
                ▷▷ doal preamble ◁◁+
n:=deg((1+gamb)^9,gamb);
```

Write the dynamics of the current finer level in terms of evolving grid values u_j:

```
                ▷▷ doal preamble ◁◁+
operator u; depend u,t;
```

The microscopic dynamics on the finer level will be some version of the following near general linear evolution $\frac{du_j}{dt} = gj$. We earlier set these coefficients and choose truncations in order to analyse different models.

```
                    ▷▷ doal preamble ◁◁+
gj:=d*(u(j+1)-2*u(j)+u(j-1))
  -c*(u(j+1)-u(j-1))/2
  +gama*cc*(u(j+2)-2*u(j+1)+2*u(j-1)-u(j-2))/2
  +gama*c2*(u(j+2)-4*u(j+1)+6*u(j)-4*u(j-1)+u(j-2))
  +gama^2*c3*(u(j+3)-6*u(j+2)+15*u(j+1)-20*u(j)
    +15*u(j-1)-6*u(j-2)+u(j-3))
  +gama^3*c4*(u(j+4)-8*u(j+3)+28*u(j+2)-56*u(j+1)
    +70*u(j)-56*u(j-1)+28*u(j-2)-8*u(j-3)+u(j-4))
  ;
```

Check the microscopic dynamics by writing in terms of centred difference and mean operators (this code works only for linear operators).

```
                    ▷▷ doal preamble ◁◁+
write
gjd:=( gj where { mu^2=>1+del^2/4, u(j)=>1,
  u(j+~k)=>(1+mu*del+del^2/2)^k when k>0,
  u(j+~k)=>(1-mu*del+del^2/2)^(-k) when k<0 } );
```

4 Initialise constructions

Notionally let the jth coarse element stretch from x_{2j-n-1} to x_{2j+n+1}. Create basis vectors $\boldsymbol{e}_i$ for the field in each element relative to the midpoint. Then express the lattice field in the jth element as $\boldsymbol{v}_j = \sum_i v_{j,i}\boldsymbol{e}_i$, so that $u_{2j+i} = v_{j,i}$. Denote the basis vectors $\boldsymbol{e}_i$ by `ee(i)` and treat multiplication as the inner product.

```
                    ▷▷ doal preamble ◁◁+
operator ee;
let { ee(~i)^2=>1, ee(~i)*ee(~j)=>0 };
```

Write the slow manifold model in terms of evolving coarser grid values $\bar{\mathbf{u}}$ where $\dot{\bar{u}}_j = G_j(\bar{\mathbf{u}}, \gamma, \bar{\gamma}) =$ ggj :

```
▷▷ doal preamble ◁◁+
operator uu; depend uu,t;
let df(uu(~k),t)=>sub(j=k,ggj);
```

The initial linear approximation to these conservative dynamics is the equilibria of a constant field in each element:

```
▷▷ doal initialise ◁◁
ggj:=0;
uj:=(for i:=-n-1:n+1 sum ee(i)*uu(j));
```

Extract the leading order operator gj1 as it is this that defines the existence and relevance of a slow manifold and empowers its construction.

```
▷▷ doal initialise ◁◁+
gj1:=(gj where gama=>0);
```

5 Iterate to construct a coarser model

Iterate until equations and coupling are satisfied to the requested order of accuracy (or too many iterates have taken place) [7].

```
▷▷ doal iterate ◁◁
it:=1$
repeat begin
  ◁◁ residuals ▷▷
  ◁◁ update ▷▷
  showtime;
end until {res,ibcr,ibcl}={0,0,0} or (it:=it+1)>19;
```

```
write Number_Iterations:=it;
```

Compute residuals of the governing difference equation. Discard wide operators $\mathcal{L}_{p+1}$ when applied near element boundaries by craftily using multiplication by appropriate power of the ordering paramater γ to do the truncation.

```
▷▷ residuals ◁◁
res:=for i:=-n:n sum ee(i)*gamaˆmax(0,abs(i)-1)*(
  -df(coeffn(uj,ee(i),1),t)
  +(gj where u(˜k)=>coeffn(uj,ee(k-j+i),1)) );
res_length:=length(res);
```

Compute residuals of the coupling conditions

$$E^{\pm 1}\bar{\delta}u_j = \bar{\gamma}E^{\pm 1}\bar{\delta}\bar{u}_j\,. \tag{5}$$

```
▷▷ residuals ◁◁+
ibcr:=uj*ee(+2)-uj*ee(0)-gamb*(uu(j+1)-uu(j));
ibcl:=uj*ee(-2)-uj*ee(0)-gamb*(uu(j-1)-uu(j));
```

To enable solving equations for the corrections to the slow mainfold we collect the names of the unknowns in the preamble:

```
▷▷ doal preamble ◁◁+
operator ud;
vars:=gd.(for i:=-n-1:n+1 collect ud(i))$
```

Combine the unknowns with the residuals to form the 'homological' equations to solve (including the amplitude condition); remember to undo the multiplication by powers of the ordering parameter γ.

```
                    ▷▷ update ◁◁
eqns:=for i:=-n:n collect (
    coeffn(res,ee(i),1)/gamaˆmax(0,abs(i)-1)
    -gd+(gj1 where u(˜k)=>ud(k-j+i)) );
eqns:=append(eqns,{ud(0)
    ,ibcr+ud(+2)-ud(0),ibcl+ud(-2)-ud(0)});
```

Solve and update the solution.

```
                    ▷▷ update ◁◁+
soln:=solve(eqns,vars);
ggj:=ggj+sub(soln,gd);
uj:=uj+sub(soln,(for i:=-n-1:n+1 sum ee(i)*ud(i)));
```

6 Renormalise to the coarser grid

First, change the time scale to that of the new coarser grid by dividing by coupling parameter $\bar{\gamma}$ (gamb). Second, evaluate for the ordering parameter of the fine grid $\gamma = 1$, to avoid the combinatorial explosion of coupling parameters at higher grid levels. Third, scale by 2 or 4 corresponding to whether the leading macroscale dynamics will be advection or diffusion respectively.

```
                    ▷▷ doal fin ◁◁
gj:=(if c=0 then 4 else 2)*sub(gama=1,ggj/gamb);
```

Then rewrite: $\bar{\gamma} \mapsto \gamma$ and $\bar{u}_j \mapsto u_j$ to complete the change of our view of the system from the fine grid to the coarser grid.

```
                    ▷▷ doal fin ◁◁+
gj:=sub(gamb=gama,(gj where uu(˜k)=>u(k)));
```

For convenience print the evolution in terms of centred mean and difference operators.

```
                    ▷▷ doal fin ◁◁+
gjd:=( gj where { mu^2=>1+del^2/4, u(j)=>1,
    u(j+~k)=>(1+mu*del+del^2/2)^k when k>0,
    u(j+~k)=>(1-mu*del+del^2/2)^(-k) when k<0 } );
```

Print this level's evolution, numerically if high enough in the multigrid hierarchy because the fractions become cumbersome.

```
                    ▷▷ doal fin ◁◁+
if level<3 then write gjd:=gjd
else begin on rounded; print_precision 5;
     write gjd:=gjd; off rounded;
end;
```

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