Projective integration of deterministic ODEs via DMD

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This is a very first stab at a good projective integration function that uses DMD.

To do

- Try examples like the modulated oscillations of 2302.09341.pdf
- Check the order of accuracy of the algorithm.
- Develop theory quantitively justifying the DMD approach.
- Develop techniques to automatically make some of the decisions about step-sizes, burst lengths, rank, and so on.
- Develop higher accuracy versions (once we have some idea about current accuracy).
- Adapt approach to algorithms for stochastic systems.

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1 projIntDMD()

Section contents

This is a basic example of projective integration of a given system of stiff deterministic odes via DMD, the Dynamic Mode Decomposition (Kutz et al. 2016).

function [xs,xss,tss]=projIntDMD(fun,x0,Ts,rank,dt,timeSteps)

Input

- fun() is a function such as $\mathtt{dxdt=fun(t,x)}$ that computes the right-hand side of the ODE $d\vec{x}/dt = f(t,\vec{x})$ where \vec{x} is a column vector, say in \mathbb{R}^n for $n \geq 1$, t is a scalar, and the result f is a column vector in \mathbb{R}^n .
- x0 is an *n*-vector of initial values at the time ts(1). If any entries in x0 are NaN, then fun() must cope, and only the non-NaN components are projected in time.
- Ts is a vector of times to compute the approximate solution, say in \mathbb{R}^{ℓ} for $\ell > 2$.
- rank is the rank of the DMD extrapolation over macroscale time-steps.
 Suspect rank should be at least one more than the effective number of slow variables.
- dt is the size of the microscale time-step. Must be small enough so that RK2 integration of the ODEs is stable.
- timeSteps is a two element vector:
 - timeSteps(1) is the time thought to be needed for microscale simulation to reach the slow manifold;
 - timeSteps (2) is the subsequent time which DMD analyses to model the slow manifold (must be longer than rank · dt).

Output

- xs, $n \times \ell$ array of approximate solution vector at the specified times (the transpose of what MATLAB integrators do!)
- xss, optional, $n \times \text{big}$ array of the microscale simulation bursts—separated by NaNs for possible plotting.
- tss, optional, 1 × big vector of times corresponding to the columns of xss.

Compute the time-steps and create storage for outputs.

```
DT=diff(Ts);
n=length(x0);
```

```
xs=nan(n,length(Ts));
xss=[];tss=[];
```

If any xO are NaN, then assume the time derivative routine can cope, and here we just exclude these from DMD projection and from any error estimation. This allows a user to have space in the solutions for breaks in the data vector (that, for example, may be filled in with boundary values for a PDE discretisation).

```
s6 j=find(~isnan(x0));
```

If either of the timeSteps are non-integer valued, then assume they are both times, instead of micro-time-steps, so set the number of time-steps accordingly (multiples of dt).

```
timeSteps=round(timeSteps/dt);
timeSteps(2)=max(rank+1,timeSteps(2));
```

Set an algorithmic tolerance for miscellaneous purposes. As at Jan 2018, it is a guess. It might be similar to some level of microscale 'noise' in the burst. Also, in an oscillatory mode for projection, set the expected maximum number of cycles in a projection.

```
algTol=log(1e8);
cycMax=3;
```

Initialise first result to the given initial condition.

```
115 xs(:,1)=x0(:);
```

Projectively integrate each of the time-steps from t_k to t_{k+1} .

```
for k=1:length(DT)
```

Microscale integration is simple, second-order, Runge–Kutta method. Reasons: the start-up time for implicit integrators, such as ode15s, is too onerous to be worthwhile for each short burst; the microscale time-step needed for stability of explicit integrators is so small that a low order method is usually accurate enough.

If user requests microscale bursts, then store.

```
if nargout>1,xss=[xss x nan(n,1)];
if nargout>2,tss=[tss Ts(k)+(0:sum(timeSteps))*dt nan];
end,end
```

Grossly check on whether the microscale integration is stable. Use the 1-norm, the largest column sum of the absolute values, for little reason. Is this any use??

```
if norm(x(j,ceil(end/2):end),1) ...
153
      > 10*norm(x(j,1:floor(end/2)),1)
154
      xMicroscaleIntegration=x, macroTime=Ts(k)
155
      warning('projIntDMD: microscale integration appears unstable')
156
      break%out of the integration loop
    end
158
    Similarly if any non-numbers generated.
    if sum(~isfinite(x(:)))>0
164
      break%out of integration loop
165
    end
```

DMD extrapolation over the macroscale But skip if the simulation has already reached the next time.

```
iFin=1+sum(timeSteps);
DTgap=DT(k)-iFin*dt;
if DTgap*sign(dt)<=1e-9
i=round(DT(k)/dt); x0(j)=x(:,i+1);
else</pre>
```

DMD appears to work better when ones are adjoined to the data vectors. ¹

```
iStart=1+timeSteps(1);
x=[x;ones(1,iFin)]; j1=[j;n+1];
```

Then the basic DMD algorithm: first the fit. However, need to test whether we need to worry about the microscale time-step being too small and leading to an effect analogous to 'numerical differentiation' errors: akin to the rule-of-thumb in fitting chaos with time-delay coordinates that a good time-step is approximately the time of the first zero of the autocorrelation.

```
[U,S,V]=svd(x(j1,iStart:iFin-1),'econ');
S=diag(S);
Sr = S(1:rank); % singular values, rx1
AUr=bsxfun(@rdivide,x(j1,iStart+1:iFin)*V(:,1:rank),Sr.');%nxr
Atilde = U(:,1:rank)'*AUr; % low-rank dynamics, rxr
[Wr, D] = eig(Atilde); % rxr
Phi = AUr*Wr; % DMD modes, nxr
```

Second, reconstruct a prediction for the time-step. The current microsimulation time is $\mathtt{dt*iFin}$, so step forward an amount to predict the systems state at $\mathtt{Ts}(\mathtt{k+1})$. Perhaps should test ω and abort if 'large' and/or positive?'? Answer: not necessarily as if the rank is large then the omega could contain large negative values.

A reason is as follows. Consider the one variable linear ode $\dot{x}=f+J(x-x_0)$ with $x(0)=x_0$ (as from a local linearisation of nonlinear ode). The solution is $x(t)=(x_0-f/J)+(f/J)e^{Jt}$ which sampled at a time-step τ is $x_k=(x_0-f/J)+(f/J)G^k$ for $G:=e^{J\tau}$. Then $x_{k+1}\neq ax_k$ for any a. However, $\begin{bmatrix} x_{k+1} \\ 1 \end{bmatrix}=\begin{bmatrix} G & a \\ 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ 1 \end{bmatrix}$ for a constant $a:=(x_0-f/J)(1-G)$. That is, with ones adjoined, the data from the ode fits the DMD approach.

Table 1: criterion for deciding if some DMD modes are to be neglected, and if not neglected then are they growing too badly?

$\operatorname{neglectness}$	range for	reason
	$\varepsilon \approx 10^{-8}$	
$\max(0, -\log_e b_i)$	0 - 19	Very small noise in the burst implies a
		numerical error mode.
$\max(0, -\Re\omega_i \Delta t)$	0 - 19	Rapidly decaying mode of the macro-
		time-step is a micro-mode that hap-
		pened to be resolved in the data.
badness		provided not already neglected
$\max(0, +\Re\omega_i\Delta t)$	0 - 19	Micro-scale mode that rapidly grows,
		so macro-step should be smaller.
$\frac{3}{C} \Im\omega_i \Delta t$	0 - 19	An oscillatory mode with $\geq C$ cycles
		in macro-step Δt .

```
omega = log(diag(D))/dt; % continuous-time eigenvalues, rx1 bFin=Phi\x(j1,iFin); % rx1
```

But we want to neglect modes that are insignificant as characterised by Table 1, or be warned of modes that grow too rapidly. Assume appropriate to sum the neglect-ness, and the badness, for testing. Then warn if there is a mode that is too bad.

```
DTgap=DT(k)-iFin*dt;
268
    negness=max(0,-log(abs(bFin)))+max(0,-real(omega*DTgap));
269
    badness=max(0,+real(omega*DTgap))+3/cycMax*abs(imag(omega))*DTgap;
270
    iOK=find(negness<algTol);</pre>
271
    iBad=find(badness(iOK)>algTol);
    if ~isempty(iBad)
273
        warning('projIntDMD: some bad modes in projection')
274
        badness=badness(iOK(iBad))
275
        rank=rank
276
        burstDt=timeSteps*dt
277
        break
278
        end
```

Scatter the prediction into the non-Nan elements of x0.

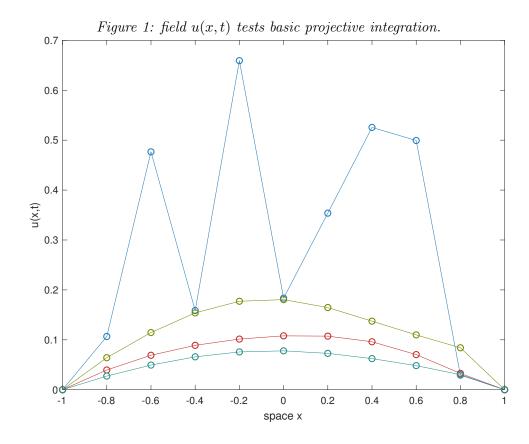
```
x0(j)=Phi(1:end-1,i0K)*(bFin(i0K).*exp(omega(i0K)*DTgap)); % nx1
```

End the omission of the projection in the case when the burst is longer than the macroscale step.

292 end

Since some of the ω may be complex, if the simulation burst is real, then force the DMD prediction to be real.

```
300 if isreal(x), x0=real(x0); end
```



xs(:,k+1)=x0;

End the macroscale time-stepping.

зов end

If requested, then add the final point to the microscale data.

if nargout>1,xss=[xss x0];
if nargout>2,tss=[tss Ts(end)];
end,end

End of the function with result vectors returned in columns of **xs**, one column for each time in **Ts**.

2 projIntDMDExample1: A first test of basic projective integration

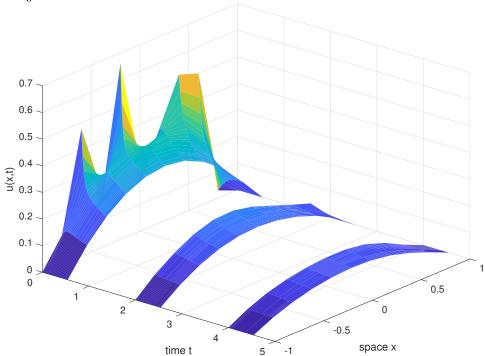
Section contents

Seek to simulate the nonlinear diffusion PDE

$$\frac{\partial u}{\partial t} = u \frac{\partial^2 u}{\partial x^2}$$
 such that $u(\pm 1) = 0$,

with random positive initial condition. Figure 1 shows solutions are attracted to the parabolic $u = a(t)(1 - x^2)$ with slow algebraic decay $\dot{a} = -2a^2$.

Figure 2: field u(x,t) during each of the microscale bursts used in the projective integration.



Set the number of interior points in the domain [-1, 1], and the macroscale time-step.

```
function projIntDMDExample1
n=9
ts=0:2:6
```

Set the initial condition to parabola or some skewed random positive values.

```
x=linspace(-1,1,n+2);
wu0=(1-x.^2).*(1+1e-9*randn(n+2,1));
u0=rand(n+2,1).*(1-x.^2);
```

Projectively integrate in time with: rank-two DMD projection; guessed microscale time-step but chosen so an integral number of micro-steps fits into a macro-step for comparison; and guessed transient time 0.4 and 7 micro-steps 'on the slow manifold'.

```
dt=2/n^2
[us,uss,tss]=projIntDMD(@dudt,u0,ts,2,dt,[0.4 7*dt])
Plot the macroscale predictions to draw Figure 1.

clf,plot(x,us,'o-')
xlabel('space x'),ylabel('u(x,t)')
%matlab2tikz('pi1Example1u.ltx','noSize',true)
%print('-depsc2',['pi1Example1u' num2str(n)])
```

Also plot a surface of the microscale bursts as shown in Figure 2.

```
tss(end)=nan;% omit the last time point
clf,surf(tss,x,uss,'EdgeColor','none')
ylabel('space x'),xlabel('time t'),zlabel('u(x,t)')
view([40 30])
print('-depsc2',['pi1Example1micro' num2str(n)])
End the main function (not needed for new enough Matlab).
end
```

The nonlinear PDE discretisation Code the simple centred difference discretisation of the nonlinear diffusion PDE with constant (usually zero) boundary values.

3 projIntDMDPatches: Projective integration of patch scheme

Section contents

As an example of the use of projective integration, seek to simulate the nonlinear Burgers' PDE

$$\frac{\partial u}{\partial t} + cu \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} \quad \text{for } 2\pi\text{-periodic } u,$$

for c = 30, and with various initial conditions. Use a patch scheme (Roberts & Kevrekidis 2007) to only compute on part of space as shown in Figure 3.

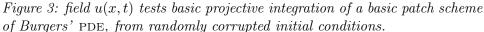
Function header and variables needed by discrete patch scheme.

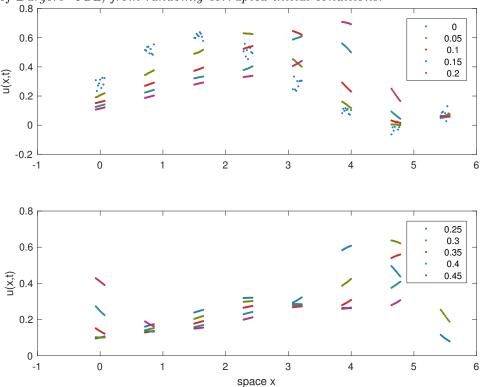
```
function projIntDMDPatches global dx DX ratio j jp jm i I
```

Set parameters of the patch scheme: the number of patches; number of micro-grid points within each patch; the patch size to macroscale ratio.

```
nPatch=8
nSubP=11
ratio=0.1
```

The points in the microscale, sub-patch, grid are indexed by i, and I is the index of the mid-patch value used for coupling patches. The macroscale patches are indexed by j and the neighbours by jp and jm.





- i=2:nSubP-1; % microscopic internal points for PDE
- I=round((nSubP+1)/2); % midpoint of each patch
- 48 j=1:nPatch; jp=mod(j,nPatch)+1; jm=mod(j-2,nPatch)+1; % patch index

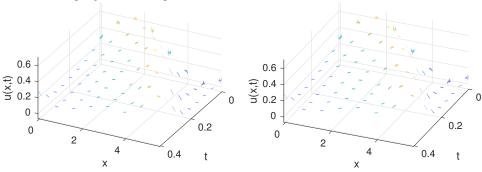
Make the spatial grid of patches centred at X_j and of half-size $h = r\Delta X$. To suit Neumann boundary conditions on the patches make the micro-grid straddle the patch boundary by setting $dx = 2h/(n_{\mu} - 2)$. In order for the microscale simulation to be stable, we should have $dt \ll dx^2$. Then generate the microscale grid locations for all patches: x_{ij} is the location of the *i*th micro-point in the *j*th patch.

```
X=linspace(0,2*pi,nPatch+1); X=X(j); % patch mid-points
DX=X(2)-X(1) % spacing of mid-patch points
dx=2*ratio*DX/(nSubP-2) % micro-grid size
dt=0.4*dx^2; % micro-time-step
x=bsxfun(@plus,dx*(-I+1:I-1)',X); % micro-grids
```

Set the initial condition of a sine wave with random perturbations, surrounded with entries for boundary values of each patch.

Set the desired macroscale time-steps over the time domain.

Figure 4: stereo pair of the field u(x,t) during each of the microscale bursts used in the projective integration.



ts=linspace(0,0.45,10) 76

> Projectively integrate in time with: DMD projection of rank nPatch + 1; guessed microscale time-step dt; and guessed numbers of transient and slow steps.

[us,uss,tss]=projIntDMD(@dudt,u0(:),ts,nPatch+1,dt,[20 nPatch*2]); Plot the macroscale predictions to draw Figure 3, in groups of five in a plot.

```
figure(1),clf
92
    k=length(ts); ls=nan(5,ceil(k/5)); ls(1:k)=1:k;
93
    for k=1:size(ls,2)
94
      subplot(size(ls,2),1,k)
      plot(x(:),us(:,ls(:,k)),'.')
96
      ylabel('u(x,t)')
97
      legend(num2str(ts(ls(:,k))'))
98
    end
99
    xlabel('space x')
100
    %matlab2tikz('pi1Test1u.ltx','noSize',true)
101
    %print('-depsc2','pi1PatchesU')
102
    Also plot a surface of the microscale bursts as shown in Figure 4.
```

```
tss(end)=nan; %omit end time-point
    figure(2),clf
114
    for k=1:2, subplot(2,2,k)
115
      surf(tss,x(:),uss,'EdgeColor','none')
116
      ylabel('x'),xlabel('t'),zlabel('u(x,t)')
117
      axis tight, view(121-4*k,45)
118
119
    %print('-depsc2','pi1PatchesMicro')
120
```

End the main function (not needed for new enough Matlab).

127 end

> Discretisation of Burgers PDE in coupled patches Code the simple centred difference discretisation of the nonlinear Burgers' PDE, 2π -periodic in

space.

```
function ut=dudt(t,u)
    global dx DX ratio j jp jm i I
    nPatch=j(end);
138
    u=reshape(u,[],nPatch);
139
    Compute differences of the mid-patch values.
    dmu=(u(I,jp)-u(I,jm))/2; % \mu\delta
    ddu=(u(I,jp)-2*u(I,j)+u(I,jm)); % \delta^2
146
    dddmu=dmu(jp)-2*dmu(j)+dmu(jm);
147
    ddddu=ddu(jp)-2*ddu(j)+ddu(jm);
148
    Use these differences to interpolate fluxes on the patch boundaries and hence
    set the edge values on the patch (Roberts & Kevrekidis 2007).
    u(end,j)=u(end-1,j)+(dx/DX)*(dmu+ratio*ddu ...
154
             -(dddmu*(1/6-ratio^2/2)+ddddu*ratio*(1/12-ratio^2/6)));
155
    u(1,j)=u(2,j)
                         -(dx/DX)*(dmu-ratio*ddu ...
156
             -(dddmu*(1/6-ratio^2/2)-ddddu*ratio*(1/12-ratio^2/6)));
157
    Code Burgers' PDE in the interior of every patch.
    ut=(u(i+1,j)-2*u(i,j)+u(i-1,j))/dx^2 ...
163
```

4 projIntDMDExplore1: explore effect of varying parameters

Section contents

164

165

Seek to simulate the nonlinear diffusion PDE

-30*u(i,j).*(u(i+1,j)-u(i-1,j))/(2*dx);

ut=reshape([nan(1,nPatch);ut;nan(1,nPatch)],[],1);

$$\frac{\partial u}{\partial t} = u \frac{\partial^2 u}{\partial x^2}$$
 such that $u(\pm 1) = 0$,

with random positive initial condition.

Set the number of interior points in the domain [-1, 1], and the macroscale time-step.

```
function projIntDMDExplore1
n=9
ts=0:2:6
dt=2/n^2
ICNoise=0.3
```

Very strangely, the results from Matlab and Octave are different for the zero noise case!???? It should be deterministic. Significantly different in that Matlab fails more often.

Figure 5: errors in the projective integration of the nonlinear diffusion PDE from initial conditions that are on the slow manifold. Plotted are stereo views of isosurfaces in parameter space: the first row is after the first projective step; the second row after the second step.

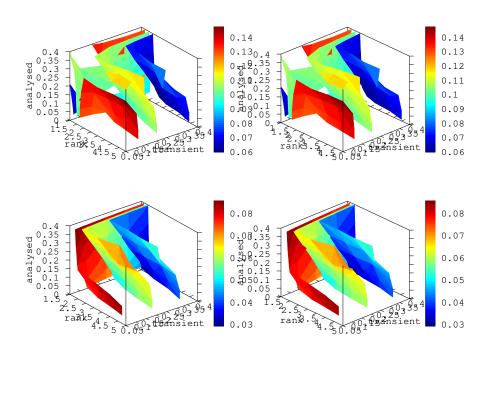


Figure 6: errors in the projective integration of the nonlinear diffusion PDE from initial conditions with noise 0.3*rand. Plotted are stereo views of isosurfaces in parameter space: the first row is after the first projective step; the second row after the second step.

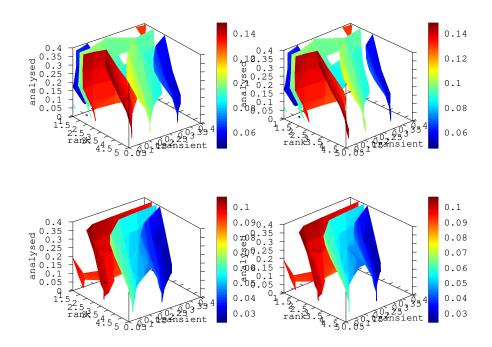


Figure 5 shows the parameter variations when the system is already on the slow manifold. The picture after two time-steps, bottom row, appears clearer than for one time-step. The errors do not vary with rank provided that it is ≥ 2 . There is only a very weak dependence upon the length of the burst being analysed—and that could be due to reduction in the gap. There is a weak dependence upon the transient-time, but only by a factor of two across the domain considered.

With the addition of a noisy initial conditions, Figure 6, the rank has an effect, and the transient-time appears to be a slightly stronger influence. I suspect this means that we need to allow the initial burst to have a longer transient time than subsequent bursts. Initial conditions may typically need a longer 'healing' time. Thus code an extra timeStep parameter.

Set the initial condition to parabola or some skewed random positive values. Without noise this initial condition is already on the slow manifold so only little reason for transient time.

```
56  x=linspace(-1,1,n+2)';
57  u0=(0.5+ICNoise*rand(n+2,1)).*(1-x.^2);
```

First find a reference solution of the microscale dynamics over all time.

[Us,Uss,Tss]=projIntDMD(@dudt,u0,ts,2,dt,[0 2]);

Set up various combinations of parameters.

```
[rank,trant,slowt]=meshgrid(1:5,[1 2 4 6 8]*0.05,[2 4 8 12 16]*dt);
    ps=[rank(:) trant(:) slowt(:)];
    Projectively integrate in time with various parameters.
    errs=[]; relerrs=[];
    for p=ps'
    [us,uss,tss]=projIntDMD(@dudt,u0,ts,p(1),dt,p(2:3));
    Plot the macroscale predictions
    if 0
87
      clf,plot(x,Us,'o-',x,us,'x--')
88
      xlabel('space x'),ylabel('u(x,t)')
      pause(0.01)
    end
91
    Accumulate errors as function of time.
    err=sqrt(sum((us-Us).^2))
    errs=[errs;err];
    relerrs=[relerrs;err./sqrt(sum(Us.^2))];
    End the loop over parameters.
    end
106
    Stereo view of isosurfaces of errors after both one and two time-steps. The
    three surfaces are the quartiles of the errors, coloured accordingly, but with a
    little extra colour from position for clarity.
    clf()
114
    vals=nan(size(rank));
115
    for k=1:2
116
      vals(:)=errs(:,k+1);
      q=prctile(vals(:),(0:4)*25)
118
      for j=1:2, subplot(2,2,j+2*(k-1)), hold on
119
         for i=2:4 % draw three quartiles
120
           isosurface(rank,trant,slowt,vals,q(i) ...
121
           ,q(i)+0.03*(rank/10-trant+slowt))
122
         end, hold off
         xlabel('rank'),ylabel('transient'),zlabel('analysed')
124
         colorbar
125
         set(gca,'view',[57-j*5,30])
126
      end%j
127
    end%k
    Save to file
    print('-depsc2',['explore1icn' num2str(ICNoise*10)])
    End the main function (not needed for new enough Matlab).
    end
143
```

The nonlinear PDE discretisation Code the simple centred difference discretisation of the nonlinear diffusion PDE with constant (usually zero) boundary values.

```
function ut=dudt(t,u)
function ut=dudt(t,u)
function ut=dudt(t,u)
function ut=dudt(t,u)
function ut=dudt(t,u)
function ut=length(u);
function ut=length(u);
function ut=dudt(t,u)
function ut=dud
```

5 projIntDMDExplore2: explore effect of varying parameters

Section contents

Seek to simulate the nonlinear diffusion PDE

$$\frac{\partial u}{\partial t} = u \frac{\partial^2 u}{\partial x^2}$$
 such that $u(\pm 1) = 0$,

with random positive initial condition.

Set the number of interior points in the domain [-1, 1], and the macroscale time-step.

```
function projIntDMDExplore2
n=9
dt=2/n^2
ICNoise=0
```

Set micro-simulation parameters. Rank two is fine when starting on the slow manifold. Choose middle of the road transient and analysed time.

```
32 rank=2
33 timeSteps=[0.2 0.2]
```

Try integrating with macro time-steps up to this sort of magnitude.

39 Ttot=9

Set the initial condition to parabola or some skewed random positive values. Without noise this initial condition is already on the slow manifold so only little reason for transient time.

```
x=linspace(-1,1,n+2)';
u0=(0.5+ICNoise*rand(n+2,1)).*(1-x.^2);
```

First find a reference solution of the microscale dynamics over all time, here stored in Uss.

```
[Us,Uss,Tss]=projIntDMD(@dudt,u0,[0 Ttot],2,dt,[0 Ttot]);
```

Projectively integrate two steps in time with various parameters. But remember that projIntDMD rounds timeSteps etc to nearest multiple of dt, so some of the following is a little dodgy but should not matter for overall trend.

```
Dts=0.1*[1 2 4 6 10 16 26]
    errs=[]; relerrs=[]; DTs=[];
69
   for p=Dts
70
    [~,j]=min(abs(sum(timeSteps)+p-Tss))
    ts=Tss(j)*(0:2)
    js=1+(j-1)*(0:2);
73
    [us,uss,tss]=projIntDMD(@dudt,u0,ts,rank,dt,timeSteps);
    Plot the macroscale predictions
    if 1
      clf,plot(x,Uss(:,js),'o-',x,us,'x--')
81
      xlabel('space x'),ylabel('u(x,t)')
82
      pause(0.01)
83
    end
84
    Accumulate errors as function of time.
    err=sqrt(sum((us-Uss(:,js)).^2))
90
    errs=[errs;err];
91
    relerrs=[relerrs;err./sqrt(sum(Uss(:,js).^2))];
    End the loop over parameters.
    end
    Plot errors
    loglog(Dts,errs(:,2:3),'o:')
    xlabel('projective time-step')
107
    ylabel('steps error')
108
    legend('one','two')
109
    grid
110
    matlab2tikz('pi1x2.ltx')
    End the main function (not needed for new enough Matlab).
    end
119
    The nonlinear PDE discretisation Code the simple centred difference
    discretisation of the nonlinear diffusion PDE with constant (usually zero)
    boundary values.
    function ut=dudt(t,u)
131
    n=length(u);
132
    dx=2/(n-1);
133
    j=2:n-1;
```

134

135

136

ut=[0

 $u(j).*(u(j+1)-2*u(j)+u(j-1))/dx^2$

137 0]; 138 end

References

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