Tools in Scientific Computing Prof. Aditya Bandopadhyay Department of Mechanical Engineering Indian Institute of Technology, Kharagpur

Lecture - 35 Reaction-Diffusion system in PETSc

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Hi guys, in this particular lecture we are going to continue on our journey of solving for the steady state distribution of this particular equation right.

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So, just to recap this is the kind of discretization we had and the Jacobian would look something like this alright.

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So, let us start coding and because it is a one dimensional problem we do not need any dm - going around over here but, we will need a one d grid something like this right.

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So, let us make a new file. So, first things first #include <petsc.h> int main(int argc, char **argv) return PetscFinalize() alright.

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So, let us save this as rxn_dfn.c just to signify its a reaction diffusion system alright. So, first things first we need to define the various things we will need. So, we are going to need a DM da.

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But in this case it will be DM and will call it da; and we are going to need a SNES about from this we are going to need AppCtx which is to hold the value of rho and all these things. So, AppCtx we will define it as user because the user is going to supplied, we are going to need two vectors one is u and one is uexact just to make a comparison we are going to need anyway.

So, let us continue on this whenever we need a new variable we will sort of declare it and we need a DMDALocalInfo for performing the loops and we will call it info.



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So, the data type DA is essentially DMDACreate1d ok.

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So, one dimensional regular array and this is the distributed array object ok. So, we going to use this DMDACreate1d and it will help us in creating the one dimensional grid alright.

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So, let us proceed so, we will need PetscInitialize we have PETSC sorry this will have one &argc, &argv, NULL and the help text alright then, we will go ahead and let us first declare what the user context will be so, we have to declare the struct so typdef struct. So, this will be double so what all things do we need so, we going to need rho we going to need M; so we going to need ρ and M we also going to need α and β just to specify the boundary conditions in terms of M alright.

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So, let us declare that and that is pretty much it. So, we will define it as AppCtx so that is the data type alright so; let us declare the data type over here so we have user.rho is equal to so what was ρ , ρ in terms of rather M was in terms of ρ right. So, let us define ρ to be 12 that way M becomes 1 so, we can do this to the 12.0 alright; user.M will be the square of user.rho/12.0, 2 well its a square so, we do not need to do this here.

Then, we need to define the α so, user.alpha will be simply user.M, user.beta will be simply 16.0*user.M so, we have defined all the parameters there are alright. So, these are what is required after initialization so, this is these are just the user defined values.

So, once we have; once we have the user defined values we will have DMDA creation so DMDACreate 1d, it will require the communicator PETSC COMM WORLD then DM_BOUNDARY_NONE. So, let me just show you the things that we require the communicator the boundary type, the dimension of the array.

So, let us declare 9 grid points its fine then what do we have number of degrees of freedom stencil width. So, number of degrees of freedom is 1 stencil width is 1 then, number of nodes on each processor we will declare it to the NULL because the PETSC will do the load balancing in case we have multiple processors and lastly we must pass the da, that is the distributed array over here ok.

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So stencil is one because we are defining the h on our own right so, this is it this is how the one dimensional grid is created then, we must do the other thing so DMSetFromOptions we have to pass da then, DMSetUp da and then we have to set up the application context.

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So, the there is a function DMSetApplicationContext. So, we must sort of tell the distributed array that whatever the variable or all the parameters are it has to be distributed over the grid. I mean it is not required for this problem, but there may be a problem with it with this would be required.

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So, we must pass to the array the address of the user defined context variables ok because, if it is not done it will not be able to see that struct that we have defined like this right ok. So, now that we have this we will create a global vector.

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So, let me show this. So, this is the command which will create a global vector on the grid da. So, it is the same as declaring the sort of associativity of u on d.

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So, DMCreateGlobalVector da and the address of u gets passed now, we will duplicate this vector Vec so we could have simply done create vector but that is ok, Duplicate u into uexact alright.

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Then, what we need to do is fetch the rather before fetching what we will do is because we need to pass this into the array so, DMDAGetLocalInfo we will get it into variable info alright. So, this is just because we going to pass info to the arrays because, we need to loop over the grid points. So, we will eventually need this ok.

So then, what should we do? So, our (Refer Time: 12:04) should consist of Create the exact solution because we will have to compare it eventually alright then, we must Create the SNES object. So, creating the SNES object will require Creating the Jacobian

as well; and it will require Creating the function callback. Well, in this case we will need all this we will need to create the function callback and we will need to create the Jacobian as well alright.

So let us first create the exact solution so, what do we need. So, let us first allocate let us first create the auxiliary Vec.

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So, to hold the nodal values we will create the auxiliary function so double *au, and *auexact.

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And then, over here we will do Vec or not Vec DMDAVecGetArray from da uexact needs to be put into auexact alright. Apart from this, what do we need? That is all; that is all that we need? In fact, we need to pause u so that we can create the initial condition so, we will make a single function which will Create the exact solution and the initial condition we can do it in one way.

So, DMDAVecGetArray from da get u and pass it to au. So, now that we have the objects or rather the we have assigned u exact to auexact and u to au we can pass them to GetInitialConditions and Get Initial and Exact; and we will pass to it the address of the info and we will pass the auxiliary matrices and we will pass the user context because, to construct the exact solution we will also need the user context.

So, what we can do is pass the address of user so, we will keep this form and create this function so Get Initial Exact. And we can copy this and copy this and we can create the function over here.

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So, the output will be Petsc Error Code. So, this is the function so, info instead of this we will have DMDALocalInfo star info, we will have double *au and double *auexact and void or in fact AppCtx *user because, we do not want to type cast it inside and we can use it directly. In case you put a void star you need to typecast it to AppCtx, we have done this in the previous example we do not need to typecast.

So, inside this we will create int i and double h that is the grid spacing, which will be 1.0 divided by the number of grid points minus 1 and the number of grid points is held inside the info so, 1.0/(info->mx - 1). So, this is the number of grids minus 1 alright. We also need double x for i going from i = info->xs; i < info->xs+info->xm; i++.

And so, where do we get this from and we have used this in one of the previous solver is basically this bit of code.

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Because we are passing the address of info we can use this kind of a link ok to address the content of the structure ok. So, now we are essentially looping over all the grid points.

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So, this is just a loop over grid points alright. So, inside this loop x the value of x = i*h that is fine and au[i] = user->alpha*(1.0-x) + user->beta*x. So, it is just an initial guess so, we are getting the initial guess inside this u array.

So, look, what is going on. We have the au array which we have passed from main alright, we have get vec array we are getting it we are passing it we are getting the initial condition inside this and then, we will put it back inside u. So finally, we need to so we need to eventually put it back.

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So, DMDA SetVecSetArray da uexact & u auexact and we need to copy this, this will be u and this will be au. So, we are fetching the initial conditions through this and then setting it back to the petsc vectors alright. So, au[i] will be equal to it is the guess. So, user->alpha*(1.0-x) + user->beta*x so, what it is? It is a linear interpolation between the end points.

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So, these are the two endpoints and I am saying its $alpha^*(1.0-x)+beta^*x$. So, 1 x is 0, the value of the guess is equal to α when the value is equal to 1 this becomes 0 so, the value is β ok. So, its like an initial sorry its like a linear interpolation. So this is the initial guess alright. So, that is the initial guess no problem. Now, we need to set the exact solution.

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auexact[i] = user->M*PetscPowReal(x+1.0, 4.0) and this is the not x+ what (Refer Time: 21:28) yeah 1 + x ok. So, this is the solution that we have over here ok.

So, that is the exact solution finally, at the end of this we must return 0 and that is all well and good. So, this is the function which creates the initial condition that we have over here. Finally, we can move on to the creation of this SNES object.

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So, it is the same protocol SNESCreate PETSC COMM WORLD comma the address of snes right, SNESSetDM so we have to tell that this particular SNES is linked to the

distributed array. So, snes sorry snes, da now, we must set the function call alright so we must set here the function callback and the Jacobian alright. So, the function has to be done locally because doing it on a grid ok. So, the way to do it is ok.



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Let me show you that functional reference snes set local function what is it. Dmda snes set local function local alright.

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So, it is a residual evaluation over a DM ok. So, because the function callback in this particular problem is in the form of a matrix which is assembled over the distr and the dmda ok so, that is why we need to do the following.

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So, we have DMDASNESSetFunctionLocal over da and we must do INSERT VALUES. So, that is the way it is dm mode function and ctx. So DM mode finally, we need to define the function as well. So, the function will be FormFunct and the user context. So now, let us go ahead and define this function local ok.

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So, PetscErrorCode what was so, it is a pointer to the function ok let is see if there is an error we can always fix it ok. So, PetscErrorCodeFormFunct and DMDA so we will have

the same type of inputs so, DMDALocalInfo star info what else do we have, we have the array so double *u in this case it is au ok.

So it is actually a local function evaluation and we have to pass the handle to that ok. So, we will rectify it later. So, the function should take as an input the info because we need to perform a loop then dmdas.

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So, we need to wait ok so, it will take the u array and the evaluation of the function.

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So, it will be double *aF and the ApplicationContext *user. So, what we need to do over here is to create the functions in the particular problem. So the functions will be where is it functions will be these things ok. So, and those will be stored in ff aF rather ok. So, int i const double because we do not want to change h this will be simply we can just make it double we are not going to change it anyway (info->mx - 1) alright.

So, we need double to store x and the reaction term or we can just hold it in x, we can define it later on we will then input these things these particular things ok. So double x what we need to do for. So, we need this same for loop to loop over all the nodes that is it then, we have if (i==0) then aF[i] = au[i] - user->alpha; else if (i == info->mx -1) that is the right hand side grid or the rather right hand side node then, aF[i] = au[i] - user->beta alright else you simply have the interior points. So, the interior points are easy.

So, what is the function? So, because it is happening locally that is why so first we need to have $x = i^*h$, which we have already defined and yep. So, aF[i] like the ith function will be in terms of the u which is on the local grid.

So, -u[i+1] + 2.0*u[i] - u[i-1] + user->rho*h*h*PetscSqrtReal(u[i]) so, that is the way we will declare the function and once it is successful we will simply return 0 ok.

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So, we have gone ahead and created this function. So, all these functions are valid for j equal to the inner node so, these are all the inner nodes. Because the residues will be

calculated for these function evaluations ok. So, we have DMDAsSetLocalFunctionSetFunctionLocal and it requires what let us see da then the PetscErrorCode no not the PetscError the InsertMode then the function handle to so, it needs the function handle.

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So, we need to give instead of giving the name of the function we need to give the Function handle. So, we will say that form funct is of the type DMDASNESFunction ok. So, this will make it pass the function handle. It should run without even declaring it like this, but anyway let us see if it does not work then we will think about it.

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Bie [dt Seach Yew	DMSNESSetJacobian
74 75 DMD	set <u>SNES</u> Jacobian evaluation function
76 77 //	Synopsis
79 DMD 80 Get	#include "petscanes.h" #include "petscam.h" DetscFeronofau (NURSSA#Jacobian(DN dm DetscFeronofode (*1)(SUFS Ver Nat Nat void*) void *rtv)
81 DMD 82 DMD 83	Not Collective
84 // 85 SNE	Input Argument
86 SNE 87 DMD 88 DMD	dm-DM to be used with <u>SNES</u> J - Jacobian evaluation function
89 // 90 //	ett- context for residual evaluation
92 93 94 95	<u>SNESSetJacobian()</u> is normally used, but it calls this function internally because the user context is actually associated with the <u>DM</u> . This makes the interface consistent regardless of whether the user interacts with a <u>DM</u> or not. If <u>DM</u> took a more central role at some later date, this could become the primary method of setting the Jacobian.
96 97 ret	See Also
C source file	DMSNESSetContext(), <u>SNESSetFunction()</u> , <u>DMSNESGetJacobian()</u> , <u>SNESSetJacobian()</u> , <u>SNESJacobianFunction</u>
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Now, let me make the Jacobian callback so, DMDASetSNESSetJacobianLocal alright. So, even this will contain da then the function callback if I remember correctly.

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De lat Sech y	DMSNESSetJacobian
74 75 D	n set <u>SNES</u> Jacobian evaluation function
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78 D 79 D 80 G	#include "petscsnes.h" #include "petscdm.h" Petscferrofde WSMESSetJacobian(DN dm, <u>PetscFerrofCode</u> (*3)(<u>SNES,Vec,Nat</u> ,Vait,void*),void *ctx)
81 L 82 D 83	Not Collective
84 / 85 S	Input Argument
86 S 87 D 88 D 89 /	dm- <u>DM</u> to be used with <u>SNES</u> J - Jacobian evaluation function etx - context for residual evaluation
90 / 91	Note
92 93 94 95 96	SNESSetJacobian() is normally used, but it calls this function internally because the user context is actually associated with the DM. This makes the interface consistent regardless of whether the user interacts with a DM or not. If DM took a more central role at some later date, this could become the primary method of setting the Jacobian.
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So, DMDAS as JacobianLocal DMDASNESSetJacobianLocal it is the same kind of function handle. So, dm then the function handle and the matrices ok.

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Actually the function handle should contain the matrices and the application context ok. So, this should contain the function handle so, FormJac and the type of the function is DMDASNES function and not function Jacobian ok. (Refer Slide Time: 33:45)



It has to give up this of that particular kind because, when you said Jacobian the Jacobian function has to be of this particular kind ok, alright.

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Then ok so apart from this, we need to pass the application context as well so, the address of user ok.

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So, then we need to create the function, but before that SNESSetFromOptions snes ok. So, now we need to create this form jack function. So, the form is the same as the above it needs one which created from scratch so, it is essentially going to return again an integer to say whether everything has run properly or not.

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51 B{	
53 int col[3];	
54 double h = 1.0/(info->mx - 1);	
55 double v[3];	
56	
57 for (i = info->xs; i < info->xs+info.xm; i++)	
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55 int main(int argc. char **argv)	
56 B(
67 DM da;	
68 SNES snes;	
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So, PetscErrorCode FormJac(DMDALocalInfo *info, double *au, Mat J, Mat P, AppCtx *user). It is the same thing, instead of passing the vector we are passing the auxiliary vector that is it that is the only difference ok, alright. So, int i and for the Jacobian we

going to have to insert three columns. So, int col[3] and they will keep on shifting depending on i we need a double h, which we can borrow from the previous code alright.

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And we going to need something which will store 3 values because, we will insert the 3 values ok. So, then we will do the for loop for so, we going to borrow the for loop alright. Now, if i == 0 so, what is the Jacobian we have already discussed this, but when i == 0 and i = n - 1 the Jacobian the diagonal element is simply going to be 1 alright.

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So, let us encode that so, if i = 0 then what should we do? v[0] = 1.0 and col [0] does not matter we can choose not to give call because it is going to be the same location as i. So, its we going to insert it at i, i. So, we going to do MatSetValues into P and we going to insert 1 row, the location of the row is i and we going to insert 1 column and the location of the column is also i that is why we do not need to bother about row.

And we going to insert v because, we going to insert only one value v [0] is sufficient and we going to do it as insert values. In fact, when i is 0 or 1 i is equal to the last row i==info->mx-1. So, when this is true then this needs to be done ok. So, we have to set the Jacobian to one now, when it is not the case else what should we do else you have to construct the 3 rows and do it ok.

So, col[0] = i-1, col[1] = i alright and col[i+1] is going to be not i+1 col[2] = i+1, these are the columns where we want to insert the values alright. Now, v[0] = -1.0, v[2] = -1.0 whereas, v[1] = 2+h*h*user->rho/(2*PetscSqrtReal(au[i])).

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So, it is going to be 2+h*h*user->rho/(2*PetscSqrtReal(u[i])) alright. So, this is the Jacobian you do not need to insert these values obviously.

So, we set then we simply do MatSetValues into P we going to insert 1 row we going to pass the address of i, we going to insert 3 values we going to pass the column address we

going to pass the values to be inserted address and insert values that is it. So, using this we have created the matrix P and we going to then have to assemble the matrix.

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So, we can borrow the program from the previous so in fact, we need this entire chunk.

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Because, either you assemble it if $J \mathrel{!=} P$ then you assemble J whatever the user has provided ok alright. So, looks good. So, this is the way you call the functions this is syntax for it and after this we have made all this we simply then solve.

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SNESSolve snes NULL put the solution in u and let us destroy whatever we had before finalizing so, VecDestroy(&uexact) then DMDestroy(&da) and SNESDestroy(&snes).

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So, let us see whether this compiles or not. So let us create a new target so, rxn_dfn alright.

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So, I have saved this lets see whether it compiles ok there is an error form jac and all this ok let us see what the issues are so ok.

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So, DMSetUp does not require the user context we just need to set up the application context. So, DMSetUp DMSetApplicationContext dm and the address of user ok.

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So, let us see if that error goes away unexpected so, have we missed semicolon somewhere ok.

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There was a small mistake this is not SetArray this should be RestoreArray.

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	Contra Cont	- 0 X .	x	
	for (i = info->xs; i < info->xs+info xm; i++)			
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0 22 12		(tion)		
1	finalyda (nataa b)			
1	#Include (perschi)	only once for each f		
4				
3		and that was the last		
4	typeder struct			
2	el double about the labor haber			
0	double rno, M, alpha, beta;			
1	-) ADDCTX;	ise -> r u		
8				
9	PetscErrorCode Get_Initial_Exact(DMDALocalInfo *info, double *au, double *auexact, AppCtx *			
	user)			
10				
11				
12	double $h = 1.0/(info->mx-1);$			
13	double x;	tion)		
14				
15	<pre>for (i = info->xs; i < info->xs+info->xm; i++) // Loop over gridpoints</pre>			
16				
17	x = i*h;			
18	<pre>au[i] = user->alpha*(1.0-x) + user->beta*x;</pre>			
19	<pre>auexact[i] = user->M*PetscPowReal(x+1.0, 4.0);</pre>	stie]		
20				
21				
22		the Property of the State		
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25	PetscErrorCode FormFunct(DMDALocalInfo *info, double *au, double *aF, AppCtx *user)	÷		
C source file	engeh: 2,400 lines: 131 Lin: 15 Cal: 41 Set: 0,10 Windows (2112) UTF-0 NS			
begundditya@DESKTOP-60JFFE1:/mnt/c/Users/Admin/Dropbox/TSC_petsc\$				
# P) Type here to search O Hz 📠 🗉 🐟 🔽 🔀 🧕 🧕 🧿 🎯	() ^ 선 부 \$ 12 년 ee _85	8 301 D	

Let me make it that is a small spelling mistake over here as well there is a small mistake over here as well.

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There is a small mistake over here as well. Well I have cleared some of the mistakes and they basically stemmed from declaring the variable inside the I mean as a function call to the declaring the variable going into the function as a u, but rather I am using u that was the error.

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So, now I will remove the error so, in the functions control ok form jac we have not returned 0.

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And what does it say x is set, but not used inside FormFunct ok.

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So, we do seem to get convergence, but now we should now check it with the analytical solution. So, let us see how we can check it so, we at the end of this function we have the solution inside u.

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So, what we must do is compare it with the exact solution. So, the exact solution was built over here. So, we will do the same thing VecAXPY(u, -1.0, uexact) and we will return the norm. So VecNorm(u, NORM_INFINITY, & errv) and the err variable has to be of kind double ok.

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The first first first and the set of the set	
74 if (J != P)	
75 8 {	
76 MatAssemblyBegin (J, MAT FINAL ASSEMBLY);	
77 MatAssemblyEnd(J, MAT FINAL ASSEMBLY);	
78	
79 return 0;	
80 -}	
81	
82	
<pre>83 int main(int argc, char **argv)</pre>	
84 4	
85 DM da;	
86 SNES snes;	
87 AppCtx user;	
88 Vec u, uexact;	<u></u> ا
89 double *au, *auexact, errv;	
90	
91 DMDALocalInfo info;	
92	
93	
94 PetscInitialize(&argc, &argv, NULL, "Solve Reaction diffusion system");	
95 // User defined values	
96 user.rho = 12.0;	
97 user.M = PetscSqr(user.rho/12.0);	
98 user.alpha = user.M;	
99 user.beta = 16.0*user.M:	
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begiraditya@DESKTOP-6DJFFE1:/mnt/c/Users/Admin/Dropbox/TSC_petsc\$	
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So, finally, we can print out the error. So, we can do a PetscPrintf it has to be done over the COMM WORLD and we will print %d, that is the number of grid points and the error as %g and this will be in info.mx, errv ok.

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So, let us recompile ok so the error appears to be 0.003 let us do a grid refinement. So, because we are we have declared the default to be 9 we can do a minus da refine 3.

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So, when we refine we get a much better norm let us do a larger refinement to see whether things are better ok.

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So, as we refine things become much better and we get conversions. So, this is the solution for some reason it says x is unused but, the fact of the matter is x is actually used I do not know why.

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It is quite weird to see that error it is not an error it is a warning, but I do not like to see that warning anyway. So, the solution is written and well can we draw the; can we draw the solution.

Well let us see, whether we have the option to draw the solution let us run it with refinement 6 monitor solution draw pause 10, we do not have x ok let us make let me start x min and now, we should be we should be able to show the ok.



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So, the solution goes from it did go from 1 to 16 ok it goes from 1 to 16 well there you have it.

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Just like this we can solve a complicated problem it is updating the solution depending on the number of iterations and its going to take a while. So, for large number of refinements we do get a solution which is well converge with respect to the exact solution.

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And in this particular lecture we have seen how to create out of a PDE in this case it was not a PDE but, in this case it was an ODE from that ODE we were able to create a sort of non-linear optimization problem, if you will we were able to construct the Jacobian of the discrete algebraic equations we were able to construct the functions of those equations and all those were done on a distributed grid.

So, do this on your own learn it by practice and you will see that all doing all this is not at all difficult; and with this I end this particular lecture I will see you again next time bye.