Introduction to High Performance Scientific Computing

Autumn, 2016

Lecture 14

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Vectorizing code

In general (Python, Fortran, Matlab,…), avoid for loops and *vectorize* calculations involving arrays.

Example:

```
In [27]: x=np.linspace(0,1,101)

In [28]: f = np.empty_like(x)

In [29]: for i in range(size(x)):
   ....:         f[i] = cos(x[i])**2
   ....:

In [30]: f = cos(x)**2
```

Vectorized version of loop

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```

Vectorized version of loop

- Vectorized code will usually be faster, sometimes *much faster*
- Exception: parallelizing Fortran code with OpenMp:
  vectorized code → loops → parallel loops

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Today

Programming example: from PDE → algorithm → serial code → parallel code

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Programming example

Task: Compute temperature distribution in a room

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Programming example

Task: Compute temperature distribution in a room

Governing equation: Heat equation (diffusion equation):

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + S(\mathbf{x}, t)$$

$$T(\mathbf{x}, t=0) = f(\mathbf{x})$$ Initial condition

Here, S is a *heat source.* Boundary conditions should also be specified as appropriate.

Problem: given the source, initial condition, and boundary conditions, solve for the temperature distribution, T(**x**,t)

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Programming example

Today: 1-D problem

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + S(x,t)$$

$$T(x, t=0) = f(x)$$ **Initial condition**

$$T(x=0,t) = a(t),\ \ T(x=1,t) = b(t)$$ **Boundary conditions**

$$0 \leq x \leq 1$$

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Programming example

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First consider steady problem, e.g., S = S(x)**,** a **and** b **are constants:**

$$\frac{\partial^2 T}{\partial x^2} + S(x,t) = 0$$ **Poisson equation**

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Programming example

First consider steady problem, e.g., S = S(x)**,** a **and** b **are constants:**

$$\frac{\partial^2 T}{\partial x^2} + S(x) = 0$$

Notes:

1. **This is an extremely simple problem, easy to write down the analytical solution**
2. **No need to use compiled language**
3. **Certainly no need to parallelize**
4. **But what about two-dimensional or three-dimensional problems?**
   - **Then, the picture changes considerably!**
5. **We are just considering the 1-D problem for illustrative purposes**

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Programming example

First consider steady problem, e.g., S = S(x), a **and** b **are constants:**

$$\frac{\partial^2 T}{\partial x^2} + S(x) = 0$$ **Poisson equation**

Numerical method:
1. Discretize the derivative:

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$ **2nd-order, centered scheme**

$$x_i = i * \Delta x, \; i = 1, 2, ..., N$$

$$(N+1) * \Delta x = 1$$

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Programming example

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With boundary conditions: $T_0 = T_a, \; T_N = T_b$

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Programming example

Equation for T_i: $\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} = -S_i$

In matrix form: AT = b

$$A = \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & \dots & 0 & 0 & 0 & 1 & -2 \end{bmatrix}, \; b = \frac{1}{\Delta x^2} \begin{bmatrix} -\Delta x^2 T_a - S_1 \\ -S_2 \\ \vdots \\ -S_i \\ \vdots \\ -S_{N-1} \\ -\Delta x^2 T_b - S_N \end{bmatrix}$$

- **In 1-D, this is just a tridiagonal system of equations**
- **Easy to solve directly (with, say, *DGTSV*)**

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Programming example

- In two or three dimensions, A loses it simple banded structure
- Then, direct solution becomes very expensive for large N
- *Iterative* methods are a popular alternative

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Programming example

- In two or three dimensions, A loses it simple banded structure
- Then, direct solution becomes very expensive for large N
- *Iterative* methods are a popular alternative
- Basic idea: rewrite Ax=b as $A_1x = A_2x + b$
- *Choose* A_1 so that it is easy to invert, then solve iterative system:
- $A_1x^{k+1} = A_2x^k + b$
  - Requires guess, x^0

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Jacobi iteration

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- *Choose* A_1 so that it is easy to invert, then solve iterative system:
- $A_1x^{k+1} = A_2x^k + b$
  - Requires guess, x^0
- *Jacobi iteration*: Choose A_1 to be diagonal matrix (main diagonal of A):

$$\frac{T_{i+1}^{k-1} - 2T_i^k + T_{i-1}^{k-1}}{\Delta x^2} = -S_i$$

$$T_i^k = \frac{\Delta x^2}{2} S_i + \frac{1}{2}\left(T_{i+1}^{k-1} + T_{i-1}^{k-1}\right)$$

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Jacobi iteration

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$$\boxed{T_i^k = \frac{\Delta x^2}{2} S_i + \frac{1}{2}\left(T_{i+1}^{k-1} + T_{i-1}^{k-1}\right)}$$

Main algorithm, easy to code!

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Jacobi iteration in Fortran

- Plan:
  - Set parameters: a, b, n, tol
  - Construct grid x_i
  - Construct source function, S(x), initialize T=T(x,t=0)
  - Iterate using formula below
    - Each iteration check if |Tk-Tk-1| < tol

$$\boxed{T_i^k = \frac{\Delta x^2}{2} S_i + \frac{1}{2}\left(T_{i+1}^{k-1} + T_{i-1}^{k-1}\right)}$$

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Jacobi iteration in Fortran

- One Fortran trick: set variables to be dimension(0:N+1)
  - x(0)=0, x(N+1)=1, T(0)=a, T(N+1)=b
  - Then, easy to compute T_1 using:

$$\boxed{T_i^k = \frac{\Delta x^2}{2} S_i + \frac{1}{2}\left(T_{i+1}^{k-1} + T_{i-1}^{k-1}\right)}$$

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Jacobi iteration in Fortran

- **One Fortran trick: set variables to be** dimension(0:N+1)
  - x(0)=0, x(N+1)=1, T(0)=a, T(N+1)=b
  - **Then, easy to compute** T_1 **using:**

$$\boxed{T_i^k = \frac{\Delta x^2}{2} S_i + \frac{1}{2}\left(T_{i+1}^{k-1} + T_{i-1}^{k-1}\right)}$$

Core part of code (see *jacobi1s.f90*):

```
do k1=1,kmax
   Tnew(1:n) = S(1:n)*dx2f + 0.5d0*(T(0:n-1) + T(2:n+1)) !Jacobi
   deltaT(k1) = maxval(abs(Tnew(1:n)-T(1:n))) !compute relative error
   T(1:n)=Tnew(1:n)    !update variable
   if (deltaT(k1)<tol) exit !check convergence criterion
end do
```

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Jacobi results

1. **Does the solution converge?**

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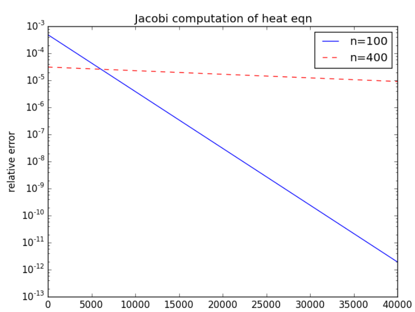
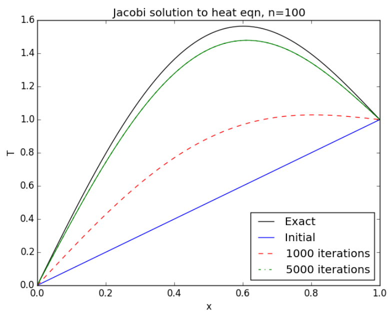
Jacobi results

1. **Does the solution converge? Yes, but very slowly for large n**



Jacobi results

1. Does it converge to the correct solution? Yes, can check that error ~ Δx^2



Jacobi results

- Jacobi is simplest, but *most inefficient* iterative solver
- Good illustration of basic ideas
- Better methods: Gauss-Seidel, SOR, conjugate gradient, multigrid

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Parallel Jacobi

Let's now parallelize the solver with OpenMP

- Look for loops that can be parallelized
- Look for vectorized operations that can be converted to loops that can be parallelized

Serial:

```
Tnew(1:n) = S(1:n)*dx2f + 0.5d0*(T(0:n-1) + T(2:n+1)) !Jacobi
deltaT(k1) = maxval(abs(Tnew(1:n)-T(1:n))) !compute relative error
```

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Parallel Jacobi

Let's now parallelize the solver with OpenMP

- **Look for loops that can be parallelized**
- **Look for vectorized operations that can be converted to loops that can be parallelized**

Parallel:

```
 dmax=0.d0
!$omp parallel do reduction(max:dmax)
do i1=1,n
    Tnew(i1) = S(i1)*dx2f + 0.5d0*(T(i1-1) + T(i1+1))
    dmax = max(dmax,abs(Tnew(i1)-T(i1)))
end do
!$omp end parallel do
deltaT(k1) = dmax
```

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Parallel Jacobi

Let's now parallelize the solver with OpenMP

- **Look for loops that can be parallelized**
- **Look for vectorized operations that can be converted to loops that can be parallelized**

Serial:

```
do i1=0,n+1
     x(i1) = i1*dx
end do
!-------------------

!set initial condition
T = (b-a)*x + a

!set source function
S = S0*sin(pi*x)
```

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Parallel Jacobi

Let's now parallelize the solver with OpenMP

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Parallel:

```
!$omp parallel do
do i1=0,n+1
    x(i1) = i1*dx
    T(i1) = (b-a)*x(i1) + a !set initial condition
    S(i1) = S0*sin(pi*x(i1)) !set source function
end do
!$omp end parallel do
```

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Parallel Jacobi notes

- **Will only see speedup with n > ~20000 (commonly seen in 2D problems)**
- **See *jacobi1s_omp.f90, jacobi1_omp.py***
- **f2py and OpenMP:** f2py --f90flags='-fopenmp' -lgomp -c jacobi1s_omp.f90 -m j1
-

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Time-dependent problem

Today: 1-D problem

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + S(x,t)$$
$$T(x,t=0) = f(x)$$
$$T(x=0,t) = a(t), \; T(x=1,t) = b(t)$$
$$0 \leq x \leq 1$$

Simple (inefficient) approach: *method of lines*

1. **Discretize spatial variable → N+2 points beteween 0 and 1**
2. **Solve resulting N ODEs with solver of choice (*odeint*, *ode15s ,…)***

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Time-dependent problem

Again, we discretize the derivative:

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$
$$x_i = i * \Delta x, \; i = 0, 1, 2, ..., N+1$$
$$(N+1) * \Delta x = 1$$

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Time-dependent problem

Again, we discretize the derivative as:

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$
$$x_i = i * \Delta x, \ i = 0, 1, 2, ..., N+1$$
$$(N+1) * \Delta x = 1$$

So, we have N ODEs:

$$\frac{dT_i}{dt} = S_i(t) + \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}, \ i = 1, 2, ..., N$$

with the boundary conditions substituted in the RHS when needed.

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Solving single ODE in python (lecture 6)

- **Use** *odeint* **from** *scipy.integrate* **module to solve:**

  $\frac{dy}{dt} = -ay$

- **Basic idea: discretize time,** t = 0, dt, …, N*dt, **and starting from** y(0) **march forward in time and compute** y(dt), … y(N*dt)
- *odeint* **chooses the stepsize,** dt, **so that error tolerances are satisfied**
- **Need to specify:**
  - **Initial condition**
  - **Timespan for integration**
  - **A Python function which provides RHS of the ODE to odeint**
- **Look at** *ode_example.py* **and lab 4**

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Time-dependent problem

Solving N ODEs:

$$\frac{dT_i}{dt} = S_i(t) + \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}, \ i = 1, 2, ..., N$$

- **Will need to provide** ***N*** **initial conditions when calling** ***odeint*.**
- **The python function which provides RHS to** ***odeint*** **will:**
  - **Take** ***t*** **and** $T_1,...,T_N$ **and any other needed parameters as input**
  - **Return** ***N*** **values for** ***dT/dt*** **as output**
- **No need for Fortran for 1D problems, but may be faster for two and three dimensions.**

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