Some Computational Science Algorithms and Data Structures

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Computational science

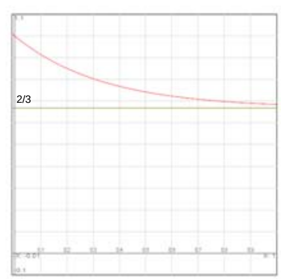
- Simulations of physical phenomena
  - fluid flow over aircraft (Boeing 777)
  - fatigue fracture in aircraft bodies
  - evolution of galaxies
  - ….
- Two main approaches
  - continuous methods: fields and differential equations (eg. Navier-Stokes equations, Maxwell's equations,…)
  - discrete methods/n-body methods: particles and forces (eg. gravitational forces)
- We will focus on continuous methods in this lecture
  - most differential equations cannot be solved exactly
  - must use numerical methods that compute approximate solutions
    - discretization: convert calculus problem to linear algebra problem
  - finite-difference, finite-element and spectral methods

Organization

- Finite-difference methods
  - ordinary and partial differential equations
  - discretization techniques
    - explicit methods: Forward-Euler method
    - implicit methods: Backward-Euler method
- Finite-element methods
  - mesh generation and refinement
  - weighted residuals
- Key algorithms and data structures
  - matrix computations
    - algorithms
      - matrix-vector multiplication (MVM)
      - matrix-matrix multiplication (MMM)
      - solution of systems of linear equations
        - » direct methods
        - » iterative methods
    - data structures
      - dense matrices
      - sparse matrices
  - graph computations
    - mesh generation and refinement

Ordinary differential equations

- Consider the ode
  $u'(t) = -3u(t)+2$
  $u(0) = 1$
- This is called an initial value problem
  - initial value of u is given
  - compute how function u evolves for t > 0
- Using elementary calculus, we can solve this ode exactly
  $u(t) = 1/3\ (e^{-3t}+2)$

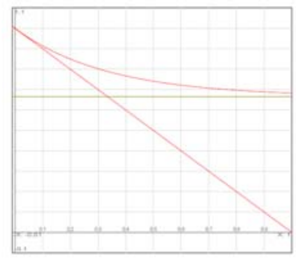


Problem

- For general ode's, we may not be able to express solution in terms of elementary functions
- In most practical situations, we do not need exact solution anyway
  - enough to compute an approximate solution, provided
    - we have some idea of how much error was introduced
    - we can improve the accuracy as needed
- General solution:
  - convert calculus problem into algebra/arithmetic problem
    - discretization: replace continuous variables with discrete variables
    - in finite differences,
      - time will advance in fixed-size steps: t=0,h,2h,3h,…
      - differential equation is replaced by difference equation

Forward-Euler method

- Intuition:
  - we can compute the derivative at t=0 from the differential equation
    u'(t) = -3u(t)+2
  - so compute the derivative at t=0 and advance along tangent to t =h to find an approximation to u(h)
- Formally, we replace derivative with forward difference to get a difference equation
  - u'(t) → (u(t+h) – u(t))/h
- Replacing derivative with difference is essentially the inverse of how derivatives were probably introduced to you in elementary calculus



Back to ode

- Original ode
  u'(t) = -3u(t)+2
- After discretization using Forward-Euler:
  (u(t+h) – u(t))/h = -3u(t)+2
- After rearrangement, we get difference equation
  u(t+h) = (1-3h)u(t)+2h
- We can now compute values of u:
  u(0) = 1
  u(h) = (1-h)
  u(2h) = (1-2h+3h^2)
  …..

Exact solution of difference equation

- In this particular case, we can actually solve difference equation exactly
- It is not hard to show that if difference equation is
  u(t+h) = a*u(t)+b
  u(0) = 1

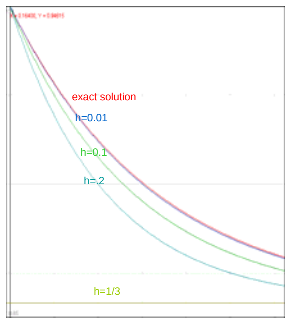
  the solution is

  u(nh) = a^n+b*(1-a^n)/(1-a)
- For our difference equation,
  u(t+h) = (1-3h)u(t)+2h

  the exact solution is
  u(nh) = 1/3((1-3h)^n+2)
- Stability:
  - values computed from difference equation will blow up if
    - ||(1-3h)|| > 1 → h > 2/3
  - for this problem, forward-Euler is stable only if step size is less than 2/3
  - in general, forward-Euler is stable only for small enough step sizes

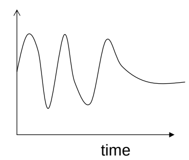
Comparison

- Exact solution
  $u(t) = 1/3\ (e^{-3t}+2)$
  $u(nh) = 1/3(e^{-3nh}+2)$ (at time-steps)
- Forward-Euler solution
  $u_f(nh) = 1/3(\ (1-3h)^n+2)$
- Use series expansion to compare
  $u(nh) = 1/3(1-3nh+9/2\ n^2h^2 \cdots + 2)$
  $u_f(nh) = 1/3(1-3nh+n(n-1)/2\ 9h^2+\ldots+2)$
  So error = $O(nh^2)$ (provided $h < 2/3$)
- Conclusion:
  – error per time step (local error) = $O(h^2)$
  – error at time nh = $O(nh^2)$



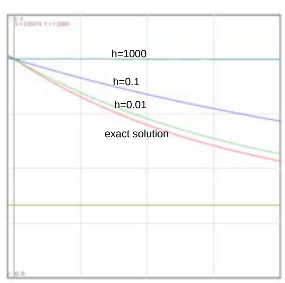
Choosing time step

- Time-step needs to be small enough to capture highest frequency phenomenon of interest
- Nyquist's criterion
  – sampling frequency must be at least twice highest frequency to prevent aliasing
  – for most finite-difference formulas, you need sampling frequencies (much) higher than the Nyquist criterion
- In practice, most functions of interest are not band-limited, so use
  – insight from application or
  – reduce time-step repeatedly till changes are not significant
- Fixed-size time-step can be inefficient if frequency varies widely over time interval
  – other methods like finite-elements permit variable time-steps as we will see later



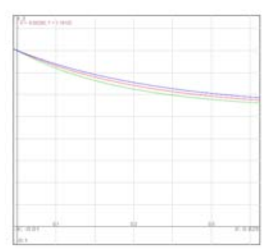
Backward-Euler method

- Replace derivative with backward difference
  $u'(t+h) \rightarrow (u(t+h) - u(t))/h$
- For our ode, we get
  $u(t+h)-u(t)/h = -3u(t+h)+2$
  which after rearrangement
  $u(t+h) = (2h+u(t))/(1+3h)$
- As before, this equation is simple enough that we can write down the exact solution:
  $u(nh) = ((1/(1+3h))^n + 2)/3$
- Using series expansion, we get
  $u(nh) = (1-3nh + (-n(-n-1)/2)\ 9h^2 + \ldots+2)/3$
  $u(nh) = (1 - 3nh + 9/2\ n^2h^2 + 9/2\ nh^2 + \ldots+2)/3$
  So error = $O(nh^2)$ (for any value of h)



Comparison

- Exact solution
  $u(t) = 1/3\ (e^{-3t}+2)$
  $u(nh) = 1/3(e^{-3nh}+2)$ (at time-steps)
- Forward-Euler solution
  $u_f(nh) = 1/3(\ (1-3h)^n+2)$
  error = $O(nh^2)$ (provided $h < 2/3$)
- Backward-Euler solution
  $u_b(n*h) = 1/3\ ((1/(1+3h))^n + 2)$
  error = $O(nh^2)$ (h can be any value you want)
- Many other discretization schemes have been studied in the literature
  – Runge-Kutta
  – Crank-Nicolson
  – Upwind differencing
  – …



Red: exact solution
Blue: Backward-Euler solution (h=0.1)
Green: Forward-Euler solution (h=0.1)

Systems of ode's

- Consider a system of coupled ode's of the form

  $u'(t) = a_{11}*u(t) + a_{12}*v(t) + a_{13}*w(t) + c_1(t)$
  $v'(t) = a_{21}*u(t) + a_{22}*v(t) + a_{23}*w(t) + c_2(t)$
  $w'(t) = a_{31}*u(t) + a_{32}*v(t) + a_{33}*w(t) + c_3(t)$

- If we use Forward-Euler method to discretize this system, we get the following system of simultaneous equations

  $u(t+h)–u(t) /h = a_{11}*u(t) + a_{12}*v(t) + a_{13}*w(t) + c_1(t)$
  $v(t+h)–v(t) /h = a_{21}*u(t) + a_{22}*v(t) + a_{23}*w(t) + c_2(t)$
  $w(t+h)–w(t) /h= a_{31}*u(t) + a_{32}*v(t) + a_{33}*w(t) + c_3(t)$

Forward-Euler (contd.)

- Rearranging, we get

  $u(t+h) = (1+ha_{11})*u(t) + ha_{12}*v(t) + ha_{13}*w(t) + hc_1(t)$
  $v(t+h) = ha_{21}*u(t) + (1+ha_{22})*v(t) + ha_{23}*w(t) + hc_2(t)$
  $w(t+h) = ha_{31}*u(t) + ha_{32}*v(t) + (1+a_{33})*w(t) + hc_3(t)$

- Introduce vector/matrix notation

  $\underline{u}(t) = [u(t)\ v(t)\ w(t)]^T$

  A = ...

  $\underline{c}(t) =[c_1(t)\ c_2(t)\ c_3(t)]^T$

Vector notation

- Our systems of equations was

  $u(t+h) = (1+ha_{11})*u(t) + ha_{12}*v(t) + ha_{13}*w(t) + hc_1(t)$
  $v(t+h) = ha_{21}*u(t) + (1+ha_{22})*v(t) + ha_{23}*w(t) + hc_2(t)$
  $w(t+h) = ha_{31}*u(t) + ha_{32}*v(t) + (1+a_{33})*w(t) + hc_3(t)$

- This system can be written compactly as follows

  $\underline{u}(t+h) = (I+hA)\underline{u}(t)+h\underline{c}(t)$

- We can use this form to compute values of $\underline{u}(h),\underline{u}(2h),\underline{u}(3h),\ldots$
- Forward-Euler is an example of explicit method of discretization
  - key operation: matrix-vector (MVM) multiplication
  - in principle, there is a lot of parallelism
    - $O(n^2)$ multiplications
    - O(n) reductions
  - parallelism is independent of runtime values

Backward-Euler

- We can also use Backward-Euler method to discretize system of ode's

  $u(t+h)–u(t) /h = a_{11}*u(t+h) + a_{12}*v(t+h) + a_{13}*w(t+h) + c_1(t+h)$
  $v(t+h)–v(t) /h = a_{21}*u(t+h) + a_{22}*v(t+h) + a_{23}*w(t+h) + c_2(t+h)$
  $w(t+h)–w(t) /h= a_{31}*u(t+h) + a_{32}*v(t+h) + a_{33}*w(t+h) + c_3(t+h)$

- We can write this in matrix notation as follows

  $(I-hA)\underline{u}(t+h) = \underline{u}(t)+h\underline{c}(t+h)$

- Backward-Euler is example of implicit method of discretization
  - key operation: solving a dense linear system $M\underline{x} = \underline{v}$
- How do we solve large systems of linear equations?

Higher-order ode's

- Higher-order ode's can be reduced to systems of first-order ode's
- Example:

  y'' + y = f(t)

  Introduce an auxiliary variable v = y'

  Then v' = y'', so original ode becomes

  v' = -y + f(t)

  Therefore, original ode can be reduced to the following system of first order ode's

  y'(t) = 0*y(t)+ v(t) + 0

  v'(t) = -y(t) + 0*v(t) + f(t)
- We can now use the techniques introduced earlier to discretize this system.
- Interesting point:
  - coefficient matrix A will have lots of zeros (sparse matrix)
  - for large systems, it is important to exploit sparsity to reduce computational effort

Intuition for system

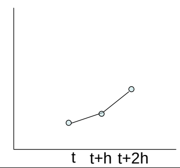
- Discretize system using forward-Euler

  y(t+h)-y(t) /h = v(t)

  v(t+h)-v(t) /h = -y(t) +f(t)
- You can eliminate v from this system to get a recurrence relation purely in terms of y

$$\frac{y(t+2h)-2y(t+h)+y(t)}{h^2} + y(t) = f(t)$$

Approximation for second derivative



Solving linear systems

- Linear system: A$\underline{x}$ = $\underline{b}$
- Two approaches
  - direct methods: Cholesky, LU with pivoting
    - factorize A into product of lower and upper triangular matrices A = LU
    - solve two triangular systems

      L$\underline{y}$ = $\underline{b}$

      U$\underline{x}$ = $\underline{y}$
    - problems:
      - even if A is sparse, L and U can be quite dense ("fill")
      - no useful information is produced until the end of the procedure
  - iterative methods: Jacobi, Gauss-Seidel, CG, GMRES
    - guess an initial approximation $\underline{x}_0$ to solution
    - error is A$\underline{x}_0$ – $\underline{b}$ (called residual)
    - repeatedly compute better approximation $\underline{x}_{i+1}$ from residual (A$\underline{x}_i$ – $\underline{b}$)
    - terminate when approximation is "good enough"

Iterative method: Jacobi iteration

- Linear system

  4x+2y=8

  3x+4y=11
- Exact solution is (x=1,y=2)
- Jacobi iteration for finding approximations to solution
  - guess an initial approximation
  - iterate
    - use first component of residual to refine value of x
    - use second component of residual to refine value of y
- For our example

  $x_{i+1} = x_i - (4x_i+2y_i-8)/4$

  $y_{i+1} = y_i - (3x_i+4y_i-11)/4$

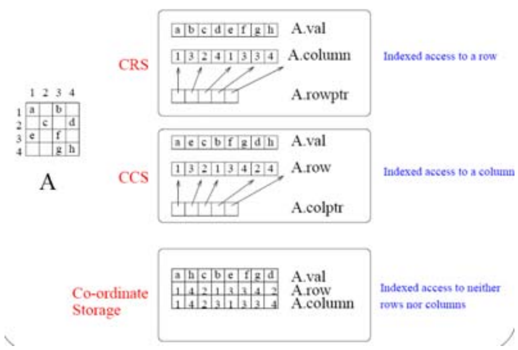
  - for initial guess (x_0=0,y_0=0)

i	0	1	2	3	4	5	6	7
x	0	2	0.625	1.375	0.8594	1.1406	0.9473	1.0527
y	0	2.75	1.250	2.281	1.7188	2.1055	1.8945	2.0396

Jacobi iteration: general picture

- Linear system Ax = b
- Jacobi iteration
  $M*x_{i+1} = (M-A)x_i + b$ (where M is the diagonal of A)
  This can be written as
  $x_{i+1} = x_i - M^{-1}(Ax_i - b)$
- Key operation:
  - matrix-vector multiplication
- Caveat:
  - Jacobi iteration does not always converge
  - even when it converges, it usually converges slowly
  - there are faster iterative methods available: CG,GMRES,..
  - what is important from our perspective is that key operation in all these iterative methods is matrix-vector multiplication

Sparse matrix representations

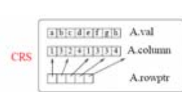


MVM with sparse matrices

- Coordinate storage

  for P = 1 to NZ do
    Y(A.row(P))=Y(A.row(P)) + A.val(P)*X(A.column(P))

- CRS storage



  for I = 1 to N do
    for JJ = A.rowptr(I) to A.rowPtr(I+1)-1 do
      Y(I)=Y(I)+A.val(JJ)*X(A.column(J)))

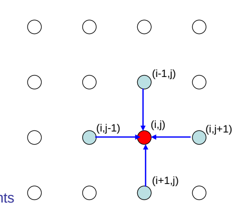
Finite-difference methods for solving partial differential equations

- Basic ideas carry over
- Example: 2-d heat equation
  $\delta^2 u/\delta x^2 + \delta^2 u/\delta y^2 = f(x,y)$
  assume temperature at boundary is fixed
- Discretize domain using a regular NxN grid of pitch h
- Approximate derivatives as differences

  $\delta^2 u/\delta x^2 =$ ((u(i,j+1)-u(i,j))/h - (u(i,j)-u(i,j-1))/h)/h
  $\delta^2 u/\delta y^2 =$ ((u(i+1,j)-u(i,j))/h - (u(i,j)-u(i-1,j))/h)/h

- So we get a system of (N-1)x(N-1) difference equations in terms of the unknowns at the (N-1)x(N-1) interior points

  $\forall$ (i,j) such that (i,j) is an interior point
  u(i,j+1)+u(i,j-1)+u(i+1,j)+u(i-1,j) – 4u(i,j) = h^2 f(ih,jh)

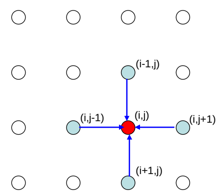


5-point stencil

Finite-difference methods for solving partial differential equations contd.)

- System of (N-1)x(N-1) difference equations in terms of the unknowns at the (N-1)x(N-1) interior points

  $\forall$ (i,j) such that (i,j) is an interior point
  u(i,j+1)+u(i,j-1)+u(i+1,j)+u(i-1,j) – 4u(i,j) = h^2 f(ih,jh)
- Matrix notation: use row-major (natural) order for u's



5-point stencil

```
 ………………………………     ….              …….
 ………………………………     u(i-1,j)        
 ………………………………     ….              
 ………………………………     u(i,j-1)        
0..1 0..0 1 -4 1 0..0 1 0…0.   u(i,j)    =  h² f(ih,jh)
0..0 0 1 0..0 1 -4 1 0..0 1 0.   u(i,j+1)     ……..
 ………………………………     …..
 ………………………………     u(i+1,j)
 ………………………………     ……
```

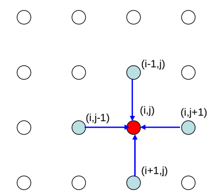
Pentadiagonal sparse matrix

Since matrix is sparse, we should use an iterative method like Jacobi.

Finite-difference methods for solving partial differential equations (contd.)

- Data structure:
  - dense matrix holding all values of u at a given time-step
  - usually, we use two arrays and use them for odd and even time-steps
- Algorithm:

  for each interior point (i,j)
  $u_{n+1}(i,j) = u_n(i,j+1)+u_n(i,j-1)+u_n(i+1,j)+u_n(i-1,j) – h^2 f(ih,jh) /4$
- Known as stencil codes
- Example shown is Jacobi iteration with five-point stencil
  - other stencils used for other problems
- Parallelism
  - all interior points can be computed in parallel
  - parallelism is independent of runtime values



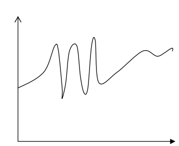
5-point stencil

Comment on Sparse MVM

- At an abstract level
  - algorithm: matrix-vector multiplication
  - data structures: four sparse representations
    - coordinate storage
    - compressed-row storage
    - compressed-column storage
    - "inlined" into code (stencil)
- Programs:
  - algorithm and data structure are intertwined, making them hard to understand for humans as well as transformation systems

Summary

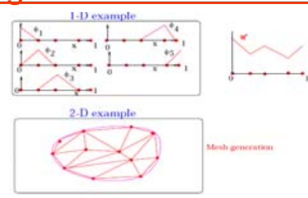
- Finite-difference methods
  - can be used to find approximate solutions to ode's and pde's
- Many large-scale computational science simulations use these methods
- Time step or grid step needs to be constant and is determined by highest-frequency phenomenon
  - can be inefficient for when frequency varies widely in domain of interest
  - one solution: structured AMR methods



Finite-element methods

- Express approximate solution to pde as a linear combination of certain basis functions
- Similar in spirit to Fourier analysis
  - express periodic functions as linear combinations of sines and cosines
- Questions:
  - what should be the basis functions?
    - mesh generation: discretization step for finite-elements
    - mesh defines basis functions ϕ_0, ϕ_1, ϕ_2,…which are low-degree piecewise polynomial functions
  - given the basis functions, how do we find the best linear combination of these for approximating solution to pde?
    - $u = \Sigma_i c_i \phi_i$
    - weighted residual method: similar in spirit to what we do in Fourier analysis, but more complex because basis functions are not necessarily orthogonal

Mesh generation and refinement



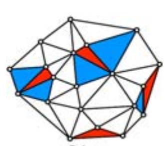
- 1-D example:
  - mesh is a set of points, not necessarily equally spaced
  - basis functions are "hats" which
    - have a value of 1 at a mesh point,
    - decay down to 0 at neighboring mesh points
    - 0 everywhere else
  - linear combinations of these produce piecewise linear functions in domain, which may change slope only at mesh points
- In 2-D, mesh is a triangularization of domain, while in 3-D, it might be a tetrahedralization
- Mesh refinement: called h-refinement
  - add more points to mesh in regions where discretization error is large
  - irregular nature of mesh makes this easy to do this locally
  - finite-differences require global refinement which can be computationally expensive

Delaunay Mesh Refinement

- Iterative refinement to remove badly shaped triangles:

```
while there are bad triangles do {
        Pick a bad triangle;
        Find its cavity;
        Retriangulate cavity;
          // may create new bad triangles
}
```

- Don't-care non-determinism:
  - final mesh depends on order in which bad triangles are processed
  - applications do not care which mesh is produced
- Data structure:
  - graph in which nodes represent triangles and edges represent triangle adjacencies
- Parallelism:
  - bad triangles with cavities that do not overlap can be processed in parallel
  - parallelism is dependent on runtime values
    - compilers cannot find this parallelism
  - (Miller et al) at runtime, repeatedly build interference graph and find maximal independent sets for parallel execution



Before

After

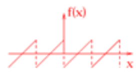
Finding coefficients

- Weighted residual technique
  - similar in spirit to what we do in Fourier analysis, but basis functions are not necessarily orthogonal
- Key idea:
  - problem is reduced to solving a system of equations $A\underline{x} = \underline{b}$
  - solution gives the coefficients in the weighted sum
  - because basis functions are zero almost everywhere in the domain, matrix A is usually very sparse
    - number of rows/columns of A ~ O(number of points in mesh)
    - number of non-zeros per row ~ O(connectivity of mesh point)
  - typical numbers:
    - A is 10^6x10^6
    - only about ~100 non-zeros per row

Finding the best choices of the coefficients:

Analogy with Fourier series:

$$f(x) = a_0 + \sum_i a_i \cos(ix) + \sum_i b_i \sin(ix)$$



How do you find 'best' choices for a's and b's?

$$\int_{-\pi}^{+\pi} f(x)\cos(kx)\,dx = \int_{-\pi}^{+\pi} \Big(a_0 + \sum_i a_i \cos(ix) + \sum_i b_i \sin(ix)\Big)\cos(kx)\,dx$$

$$= \int_{-\pi}^{+\pi} a_k \cos(kx)\cos(kx)\,dx$$

$$= a_k \pi$$

Key idea:
- residual $f(x) - a_0 + \sum_i a_i \cos(ix) + \sum_i b_i \sin(ix)$
- weight residual by known function and integrate to find corresponding coefficient

Weighted Residual Technique:

Residual: $(L u^* - f) = (L(\sum_i^N c_i \phi_i) - f)$

Weighted Residual $= (L(\sum_i^N c_i \phi_i) - f)\ \phi_k$

Equation for k^{th} unknown: $\int_\Omega \phi_k * (L(\sum_i^N c_i \phi_i) - f)\, dV = 0 \quad \Rightarrow$

If the differential equation is linear:

$$c_1 \int_\Omega \phi_k * L\phi_1\, dV + \dots + c_N \int_\Omega \phi_k * L\phi_N\, dV = \int_\Omega \phi_k f\, dV$$

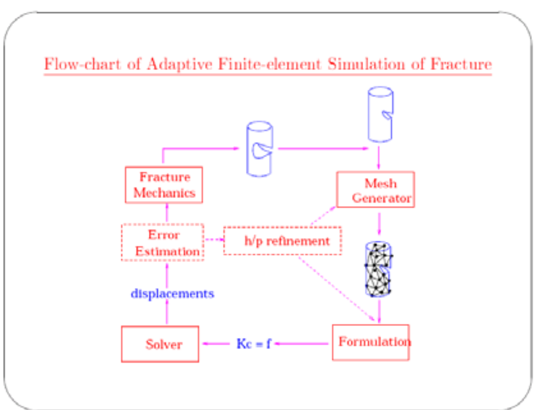
$k = 1,2,\dots N$

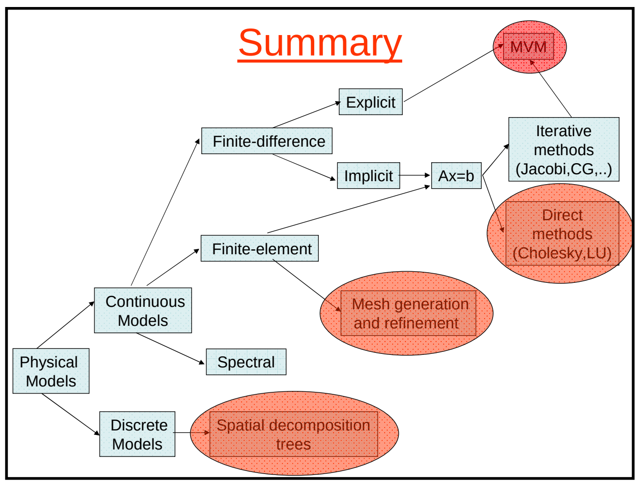
This system can be written as

$Kc = b$ where

$$K(i,j) = \int_\Omega \phi_i * L\phi_j\, dV \qquad b(i) = \int_\Omega \phi_i f\, dV$$

Key insight: Calculus problem of solving pde is converted to linear algebra problem of solving $Kc = b$ where K is sparse





Summary (contd.)

- Some key computational science algorithms and data structures
  - MVM:
    - source: explicit finite-difference methods for ode's, iterative linear solvers, finite-element methods
    - data structures: both dense and sparse matrices
  - stencil computations:
    - source: finite-difference methods for pde's
    - data structures: dense matrices
  - A=LU:
    - terminology: direct methods for solving linear systems, factorization
    - source: boundary-element methods
    - data structures: usually only dense matrices
    - comment: high-performance factorization codes use MMM as a kernel
  - mesh generation and refinement
    - source: finite-element methods
    - data structures: graphs

Summary (contd.)

- Terminology
  - regular algorithms:
    - dense matrix computations like MVM, A=LU, stencil computations
    - parallelism in algorithms is independent of runtime values, so all parallelization decisions can be made at compile-time
  - semi-regular algorithms:
    - sparse matrix computations like MVM, A=LU
    - parallelization decisions can be made at runtime once matrix is available, but before computation is actually performed
    - inspector-executor approach (see later)
  - irregular algorithms:
    - graph computations like mesh generation and refinement
    - parallelism in algorithms is dependent on runtime values
    - most parallelization decisions have to be made at runtime during the execution of the algorithm