Simulation and High-Performance Computing

Summary and Conclusion

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Day 1: Timestepping Methods

Examples:

- Mass-spring system
- Gravity
- Wave equation
- Predator-prey model

Simple timestepping:

- Explicit Euler based on forward difference
- Implicit Euler based on backward difference
- Runge based on central difference
- Leapfrog based on central difference
- Crank-Nicolson based on forward and backward difference

Day 2: Higher-order Methods

Polynomial approximation:

- Interpolation
- Numerical differentiation
- Numerical integration
- Extrapolation

Higher-order timestepping:

- Runge-Kutta methods
- Multistep methods

Day 3: Finite Difference Methods

Finite difference method:

- Grids and grid functions
- Difference quotients, discrete Laplace operator
- Method of lines
- Solving the resulting ODEs, CFL condition

Direct solvers:

- LU factorization
- Triangular matrices
- Matrices, vectors, arrays, pointers
- BLAS

Day 4: Iterative Solvers

Iterations:

- Newton iteration
- Quadratic convergence
- Power iteration
- Inverse iteration
- Rayleigh quotient

Krylov space methods:

- Minimization problem
- Gradient iteration
- Conjugate gradients
- Krylov spaces

Day 5: Algorithms for Large Systems

Multigrid iteration:

- Richardson iteration, relaxation methods
- Smoothing
- Prolongation and restriction
- Multigrid iteration

Cluster algorithm:

- Low-rank approximation, interpolation
- Cluster tree
- Forward transformation
- Recursive approximation
- Symmetric algorithm

Day 6: Shared-Memory Parallelization

OpenMP:

- Teams of threads
- Private and shared variables
- Work sharing
- Synchronization

Tasks:

- Task creation
- Waiting for tasks
- Dependencies
- Example: Block algorithms

Day 7: Vectorization

Implementation:

- Automatic vectorization
- Helping the compiler
- Explicit vectorization

Challenges:

- Data-dependant branches
- Memory bandwidth
- Latency vs throughput

Day 8: GPU Computing

Implementation:

- SIMT
- CUDA and OpenCL
- Threads, warps, thread blocks
- Graphics memory

Refinements:

- Unified memory
- Concurrent computation and memory transfer
- Shared memory

Day 9: Distributed Computing

Point-to-point communication:

- Messages and communicators
- Send and receive
- Blocking and non-blocking communication

Collective communication:

- Broadcast and reduce
- Scatter and gather
- All-to-all
- One-sided communication

Conclusion

Approximation:

- Timestepping for ODEs
- Finite differences for PDEs
- Cluster algorithms for non-local interactions

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Solution:

- LU factorization for simple systems
- Conjugate gradient method for symmetric positive definite systems
- Multigrid for large systems

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Solution:

- LU factorization for simple systems
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Implementation:

- Vectorization / GPU
- Shared-memory parallelization
- Distributed computing