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ST 2010

Scientific Computing II

Final Exam, July 21, 2010

A handwritten sheet of paper (size A4, front and back page) may be used during the exam as mnemonic. No other material is allowed. The exam is to be solved within 60 minutes, and the answers are to be written in German or English. Please try to answer all parts of the questions precisely and briefly (mind the number of credits assigned to a question). For passing the exam you will need $16,5$ out of $40 + 6$ credits. The exam consists of four problems on four pages.

1 Iterative Solvers

($\approx$ 14 credits)
Given is a 6×6 grid whose vertices are enumerated lexicographically. We apply the stencil from below to this grid.

$$\begin{bmatrix} -1 & -2 & -1 \\ -2 & 12 & -2 \\ -1 & -2 & -1 \end{bmatrix}$$

1. Assemble the matrix explicitly. No formulas required, sketch of complete matrix structure, size, and its entries is sufficient.
   ($\approx$ 4 credits)
2. What are the cost of an LU decomposition for such a system (for any grid size, i.e. arbitrary matrix size N)? (with short reasoning, no details)
   ($\approx$ 2 credits)
3. If you implement an LU decomposition, what does in-situ mean? Is in-situ well-suited for an LU decomposition of such a stencil?
   ($\approx$ 2 credits)
4. What is a well-suited colouring for the matrix from above? Sketch the structure of the matrix, if you replace the lexicographic enumeration by the coloured enumeration.
   ($\approx$ 4 credits)
5. What happens, if you replace the 12 in the stencil by 8?
   ($\approx$ 2 credits)

2 Multigrid

($\approx$ 10 credits)
Given is a $1d$ PDE problem that we solve with a multigrid solver. The solver's operators are

$$A = \begin{bmatrix} 0 & 1 & -1 \end{bmatrix} \qquad \text{and} \qquad P = \begin{bmatrix} \frac{1}{2} & 1 & \frac{1}{2} \end{bmatrix}$$

with A being the PDE's stencil and P defining the prolongation operator. We apply standard $1:2$ coarsening.

1. What is the smoothing property of a solver?
   ($\approx$ 2 credits)
2. What is a two-grid algorithm? Sketch the important basic steps.
   ($\approx$ 2 credits)
3. What is a Galerkin multigrid algorithm, i.e. how do you usually assemble the coarse-grid operator/matrix A_{2h}? Give a formula only using well-defined matrices/operators.
   ($\approx$ 1 credit)
4. Derive the Galerkin coarse-grid stencil for the matrix A_{2h} for this particular problem.
   ($\approx$ 3 credits)
5. What problems/drawbacks might arise with this coarse-grid operator—in particular if you compare this operator with the simple operators studied in the lecture? Mention two issues with a corresponding reasoning.
   ($\approx$ 2 credits)

3 Molecular Dynamics

($\approx$ 13 credits)
We study a standard molecular dynamics code with n molecules describing the overall system.

1. What is ab-initio molecular dynamics? What consequence arises if you do not use ab-initio molecular dynamics?
   ($\approx$ 2 credits)
2. Given a two-body potential, how does the movement of the molecules depend on the underlying model of the potential? Describe the link/sketch the equations.
   ($\approx$ 3 credits)
3. In molecular dynamics, one of the first steps is to build a physical model of the real world problem. One of these models is the Lennard-Jones 12-6 potential

   $$U_{LJ}(r_{ij}) = 4\epsilon \left(\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right),$$

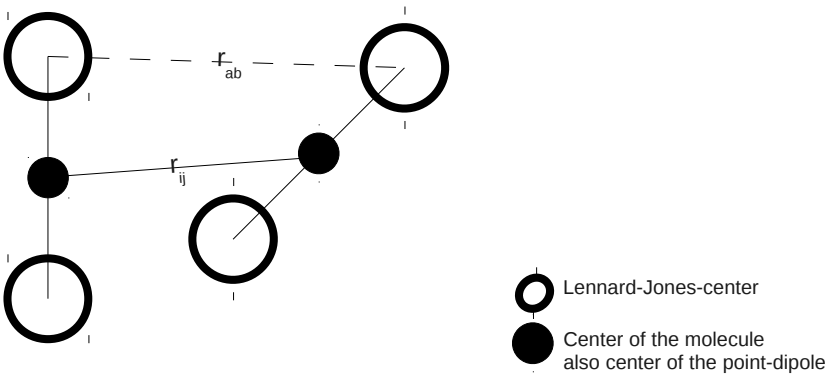
   which is composed of two parts, one of them is responsible for attraction and the other one for repulsion. Sketch the Lennard-Jones 12-6 potential graphically. Shortly describe and justify

which part of the potential has which effect on the two involved molecules. Give two examples of forces on molecules which can't be modeled using the Lennard-Jones 12-6 potential.
($\approx$ 4 credits)

4. For short-range potentials, it is sufficient to evaluate only the interactions of "neighbouring" molecules. Define the term "neighbouring" and describe the idea of the linked-cell algorithm for the efficient evaluation of short-range forces.
($\approx$ 2 credits)
5. Consider a simulation using the linked-cell algorithm and an explicit Euler for the time integration. How many force calculations do you need for the sequential code? How many force calculations do you need, if the same simulation is executed in parallel on several compute nodes? Why?
($\approx$ 2 credits)

4 2-Center-Lennard-Jones-Dipole

($\approx$ 9 credits)
To realistically simulate Carbon-Monoxide (CO) in 3d, we need a model which considers 2 Lennard-Jones-centers as well as a partial charge. The resulting potential is the 2-Center-Lennard-Jones-Dipole (2CLJD), which is composed of two identical Lennard-Jones sites, plus a point dipole μ placed in the geometric center of the molecule.



The contribution of the Lennard-Jones part is calculated via

$$U_{LJ}(r_{ij}) = \sum_{a=1}^{2}\sum_{b=1}^{2} 4\epsilon \left(\left(\frac{\sigma}{r_{ab}}\right)^{12} - \left(\frac{\sigma}{r_{ab}}\right)^{6} \right),$$

The dipolar part of the intermolecular interaction is given by

$$U_D\left(r_{ij}, \mu_i, \mu_j, \theta_a, \theta_b\right) \quad = \quad -\frac{\mu_i \mu_j \cdot f(\theta_a, \theta_b)}{r_{ij}^3},$$

where μ_i and μ_j denote the dipolar moment of molecules i and j, and $f(\theta_a, \theta_b)$ is a function representing the spatial alignment of the two molecules.

1. Of what type is the 2CLJD potential? Is it a short or long range potential? Give a short reasoning.
   ($\approx$ 3 credits)
2. Consider the interaction of two molecules of the same type: how does this interaction take place (i.e. which centers interact with each other)? How is the total force which is effective on one molecule computed from the forces of the center-center interaction?
   ($\approx$ 3 credits)
3. How can you evaluate the two different parts of the potential? Sketch implementation possibilities!
   ($\approx$ 3 credits)