Parallel Numerical Algorithms

Chapter 14 – Other Numerical Problems

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Outline

Nonlinear Equations

Potential sources of parallelism in solving nonlinear equation $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$ include

- Evaluation of function $\boldsymbol{f}$ and its derivatives in parallel
- Parallel implementation of linear algebra computations (e.g., solving linear system in Newton-like methods)
- Simultaneous exploration of different regions via multiple starting points (e.g., if many solutions are sought or convergence is difficult to achieve)

Optimization

Sources of parallelism in optimization problems include

- Evaluation of objective and constraint functions and their derivatives in parallel
- Parallel implementation of linear algebra computations (e.g., solving linear system in Newton-like methods)
- Simultaneous exploration of different regions via multiple starting points (e.g., if global optimum is sought or convergence is difficult to achieve)
- Multi-directional searches in direct search methods
- Decomposition methods for structured problems, such as linear, quadratic, or separable programming

Numerical Integration

Potential sources of parallelism in computing definite integrals include

- Evaluation of integrand function in parallel
- Partitioning of domain of integration into subdomains over which integral is computed separately in parallel
- Divide-and-conquer parallelism in adaptive quadrature (load balancing may be challenging)
- Monte Carlo method for higher dimensional integrals, with multiple random trials in parallel (requires parallel independent streams of random numbers)

Ordinary Differential Equations

Minor potential sources of parallelism in solving initial value problem for system of ODEs $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$ include

- For multi-stage methods (e.g., Runge-Kutta), computation of multiple stages in parallel
- For multi-level methods (e.g., extrapolation), computation of multiple levels (e.g., with different step sizes) in parallel
- For multi-rate methods, integration of slowly and rapidly varying components of solution in parallel

Ordinary Differential Equations

Major potential sources of parallelism in solving initial value problem for system of ODEs $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$ include

- Evaluation of right-hand-side function $\boldsymbol{f}$ in parallel (e.g., evaluation of forces for n-body problems)
- Parallel implementation of linear algebra computations (e.g., solving linear system in Newton's method for stiff ODEs)
- Partitioning equations in system of ODEs into multiple tasks (e.g., waveform relaxation, discussed next)

Picard Iteration

- Consider initial value problem for system of n ODEs $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$, $t \ge t_0$, with IC $\boldsymbol{y}(t_0) = \boldsymbol{y}_0$
- Starting with $\boldsymbol{y}_0(t) \equiv \boldsymbol{y}_0$, *Picard iteration* is given by

$$\boldsymbol{y}_{k+1}(t) = \boldsymbol{y}_0 + \int_{t_0}^{t} \boldsymbol{f}(s, \boldsymbol{y}_k(s))\, ds$$

- If $\boldsymbol{f}$ satisfies Lipschitz condition, then Picard iteration converges to solution of IVP
- Convergence may be slow, but parallelism is excellent, as problem decouples into n independent 1-D quadratures

Waveform Relaxation

- Picard iteration is simple fixed-point iteration on function space
- Picard iteration is often too slow to be useful, but other such iterations may be more rapidly convergent
- Iterative methods of this type are commonly called *waveform relaxation*

Jacobi Waveform Relaxation

- For $n = 2$, consider iteration

$$\begin{bmatrix} y_1^{(k+1)}(t) \\ y_2^{(k+1)}(t) \end{bmatrix}' = \begin{bmatrix} f_1(t, y_1^{(k+1)}(t), y_2^{(k)}(t)) \\ f_2(t, y_1^{(k)}(t), y_2^{(k+1)}(t)) \end{bmatrix}$$

- System of two independent ODEs can be solved in parallel
- Method generalizes in obvious way to arbitrary system of n ODEs and decouples system into n independent ODEs
- Because of its analogy to Jacobi iteration for linear algebraic systems, method is called *Jacobi waveform relaxation*

Gauss-Seidel Waveform Relaxation

- Convergence rate of Jacobi waveform relaxation is improved by *Gauss-Seidel waveform relaxation*, illustrated here for $n = 2$

$$\begin{bmatrix} y_1^{(k+1)}(t) \\ y_2^{(k+1)}(t) \end{bmatrix}' = \begin{bmatrix} f_1(t, y_1^{(k+1)}(t), y_2^{(k)}(t)) \\ f_2(t, y_1^{(k+1)}(t), y_2^{(k+1)}(t)) \end{bmatrix}$$

- Unfortunately, system is no longer decoupled, so parallelism is lost unless components are reordered, analogous to red-black or multicolor ordering
- More generally, multi-splittings can further enhance parallelism in waveform relaxation methods

Boundary Value Problems for ODEs

Potential sources of parallelism in solving boundary value problems for ODEs include

- For finite difference and finite element methods, parallel implementation of resulting linear algebra computations (e.g., cyclic reduction for tridiagonal systems)
- Multi-level methods
- Multiple shooting method

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