Current development work on ChemApp and SimuSage

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GTT-Technologies' 15th Annual Workshop, Herzogenrath, Germany, July 3-5, 2013

Topics

- ChemApp
  - Semi-automatic charge balance correction
- SimuSage
  - Adding Nomad
  - Lazarus port

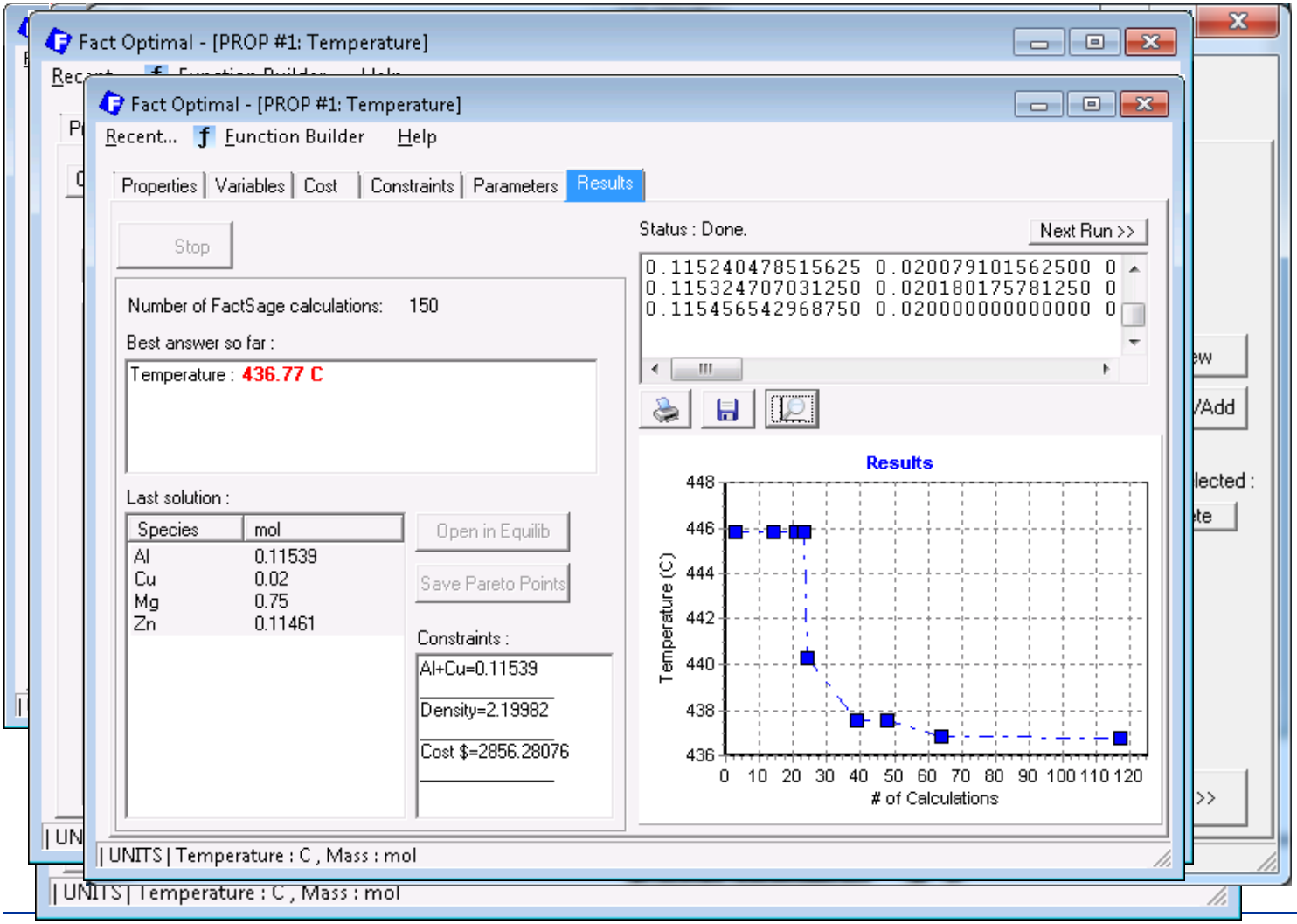
Semi-automatic charge balance correction

- The situation:
  - In iterative calculations (input to an equilibrium calculation is based on the output of a previous equilibrium calculation) electroneutrality in phases with phase-internal electrons might not be given.
  - Typical reason: rounding errors
  - Primarily a problem when “streams” are used (as opposed to “global conditions”)
  - Solution: enable the user to specify that ChemApp should set the amount of phase-internal electrons to zero before an equilibrium calculation

New subroutine: TQCONF

- `CALL TQCONF('E', 0, 0, 0, NOERR)`
  - Sets amounts of all system components with names starting with ‘e(’, ‘E(’, or ‘EA’ to zero
- `CALL TQCONF('E', I, 0, 0, NOERR)`
  - Sets amount of system component `I` (`I` begin an electron) to zero

NOMAD in FactOptimal



NOMAD

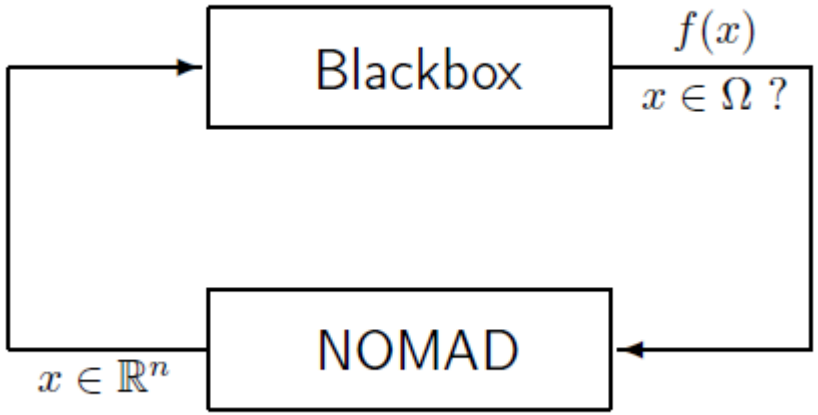
- Nonlinear Optimization by Mesh Adaptive Direct Search
- C++ implementation of the Mesh Adaptive Direct Search (MADS) algorithm*
- Designed for constrained optimization blackbox functions in the form:

$$\min_{x \in \Omega} f(x)$$

* Auded, C., and Dennis, J. (2006). Mesh Adaptive Direct Search Algorithm for Constrained Optimization. SIAM J. Opt. 17, 1, 188-217

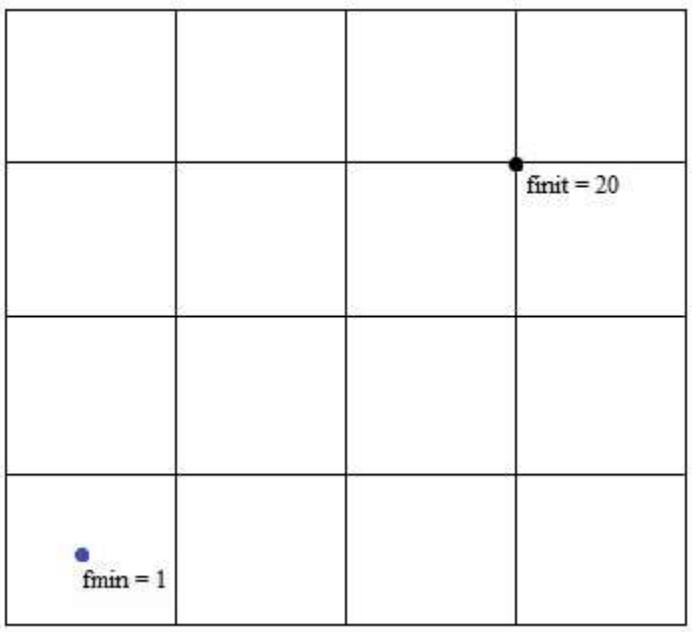
Blackbox Problems

- Unknown internal structure of the target problem
- Function can have unreliable properties
- NOMAD is intended for time-consuming blackbox simulations with a small number of variables



MADS Algorithm

- Mesh Adaptive Direct Search



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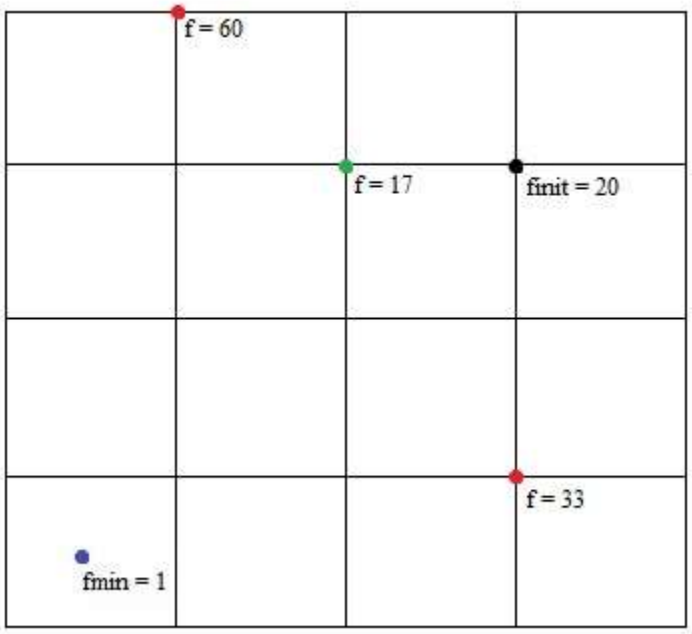

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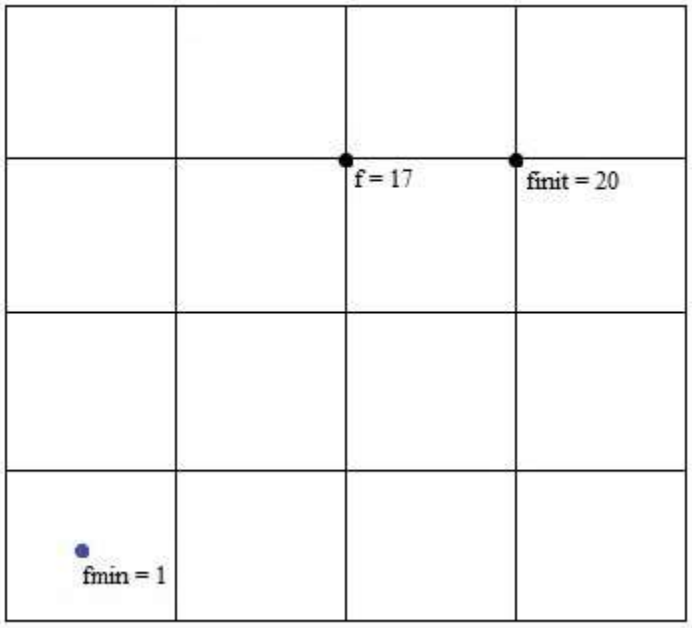

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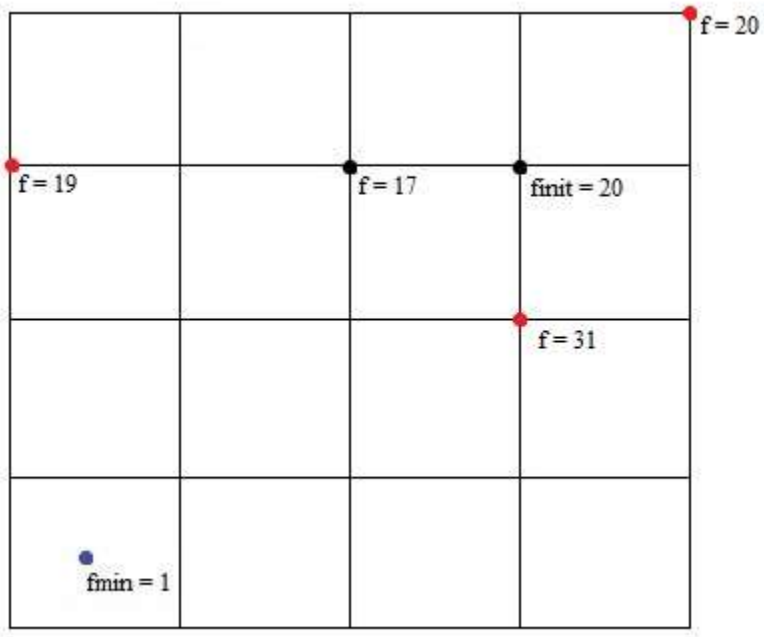

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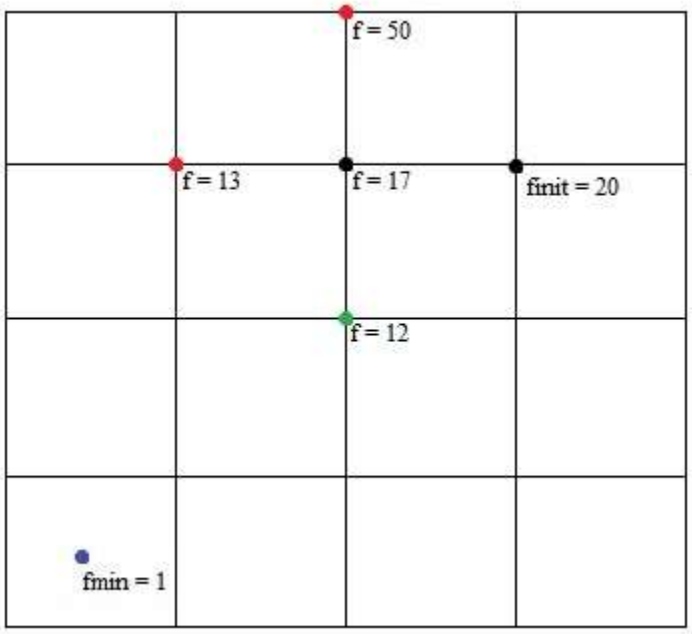

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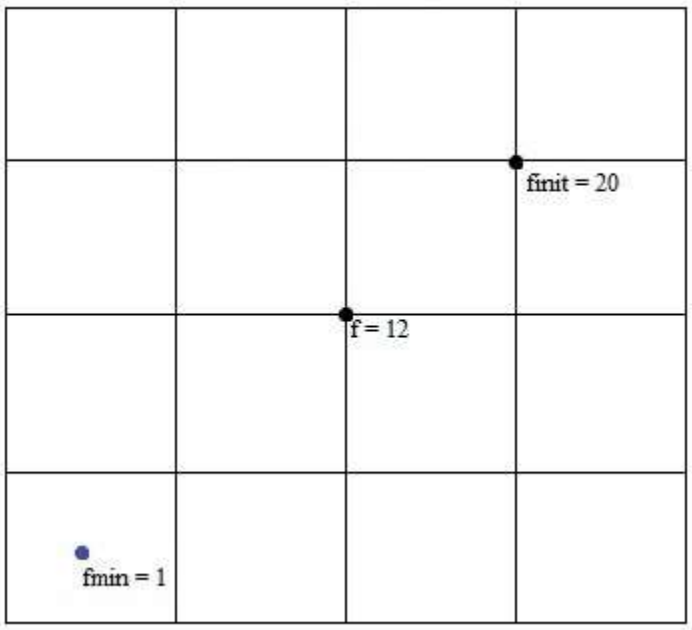

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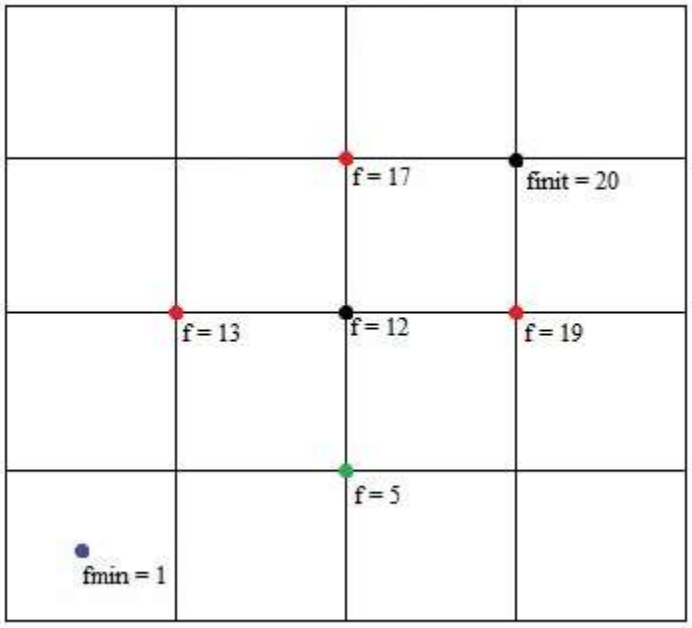

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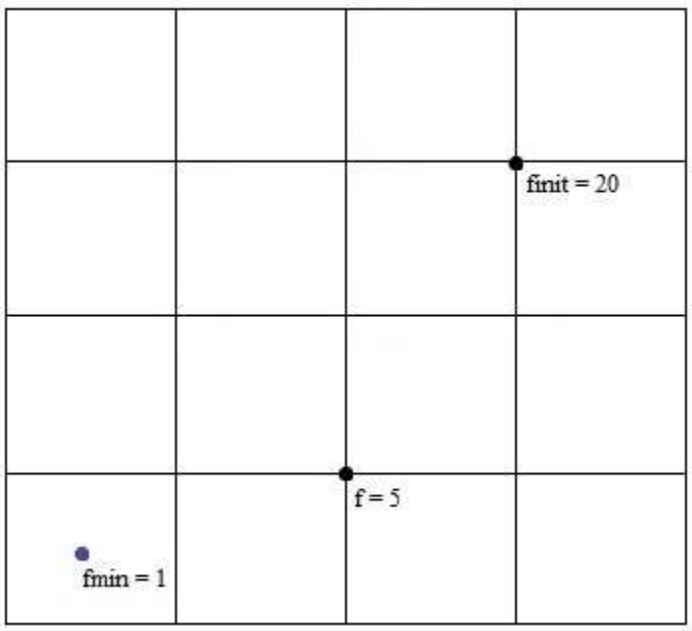

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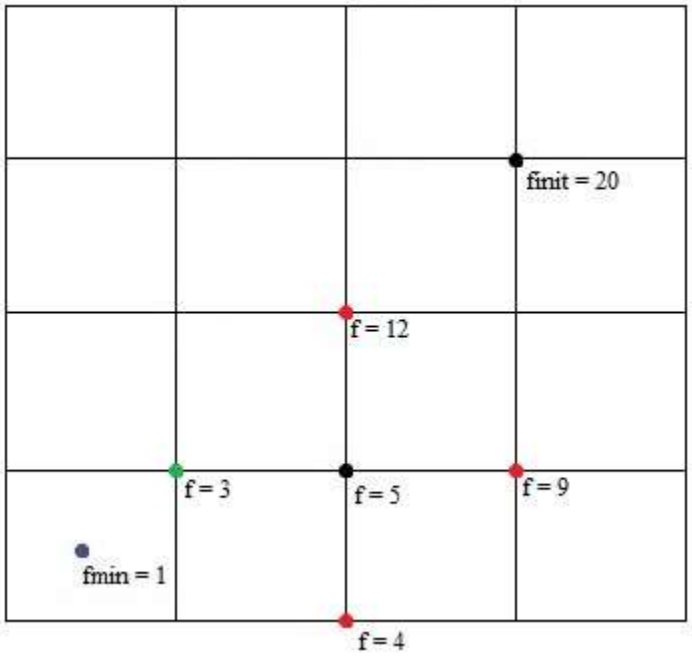

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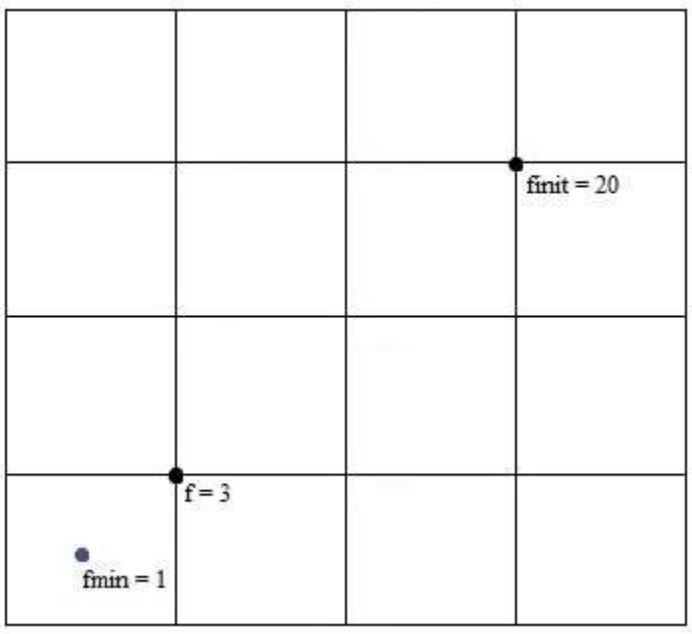

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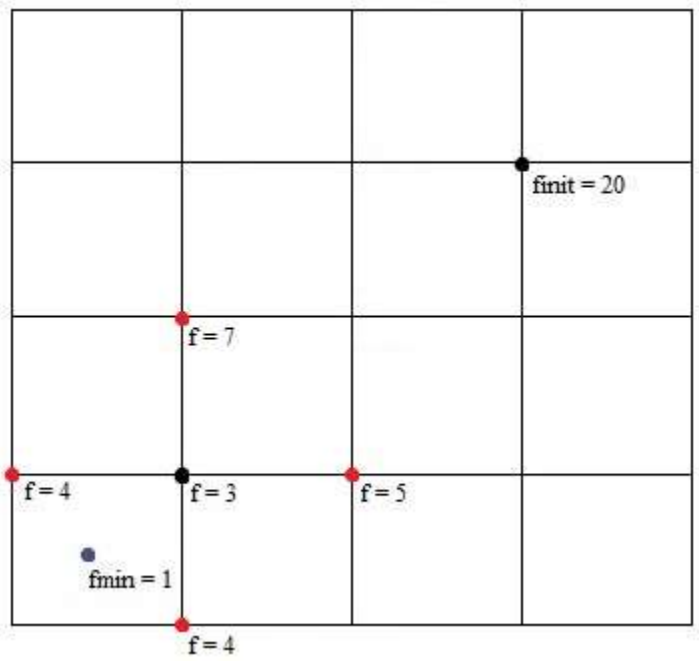

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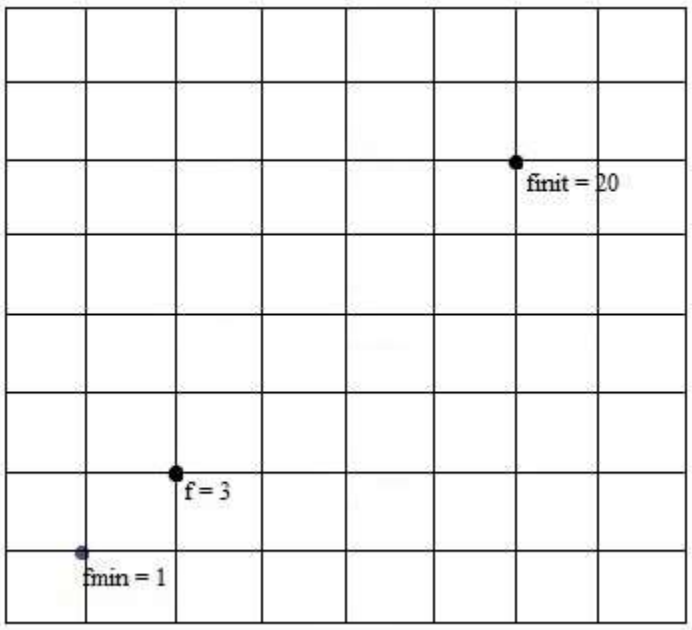

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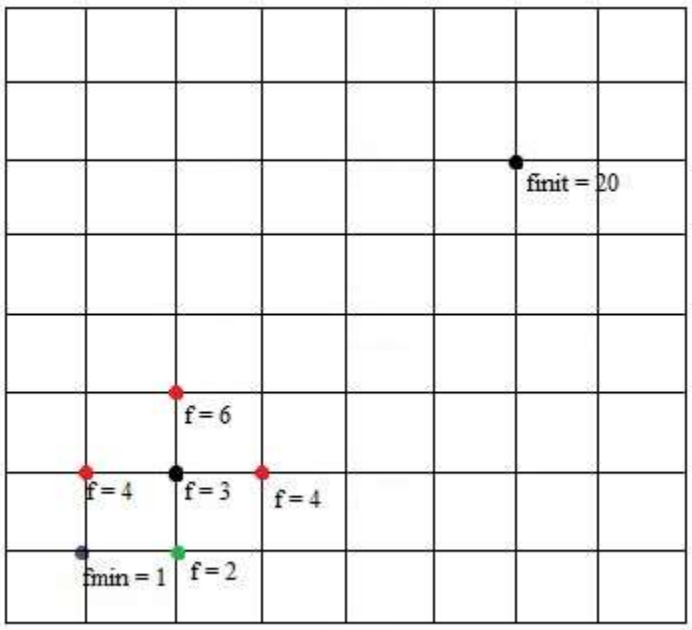

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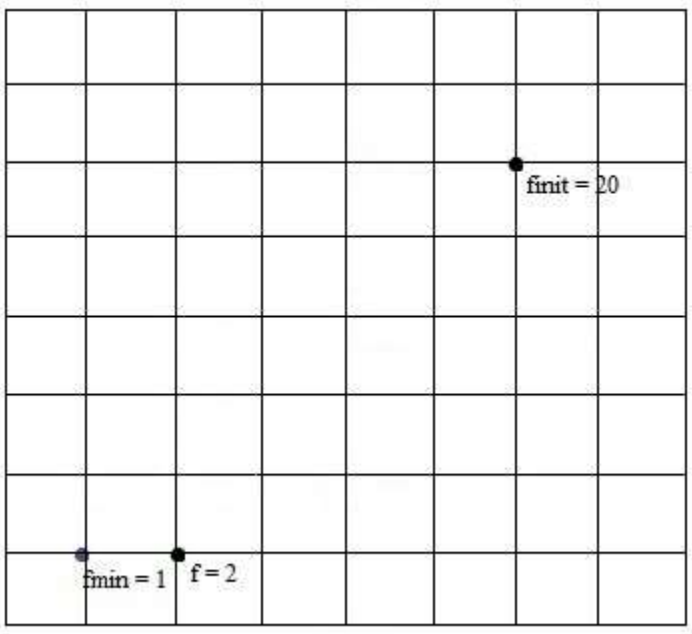

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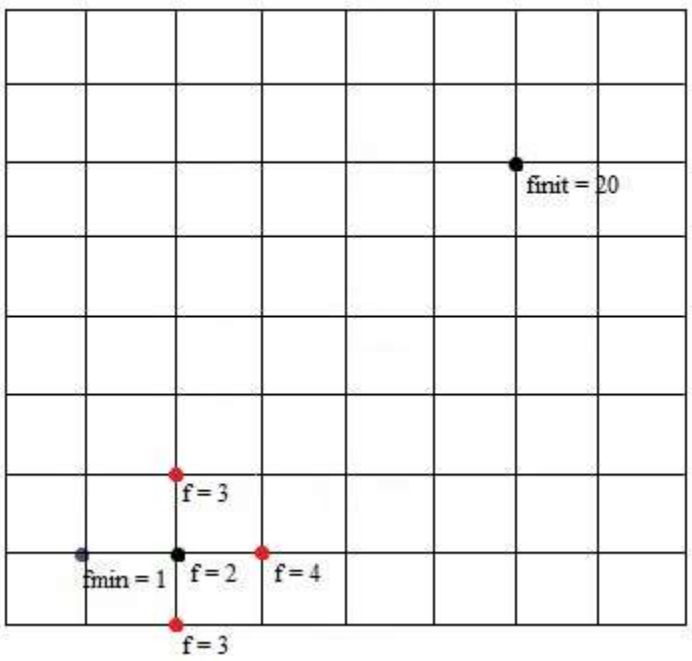

Some examples…

Thank you for your attention!