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Subject: Re: Force Field

Posted by [Kenneth P. Bowman](#) on Wed, 14 Sep 2005 02:13:28 GMT

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In article <1126634205.227520.96190@f14g2000cwb.googlegroups.com>, "Andres" <panblosky@gmail.com> wrote:

> Hi all,  
>  
> I have a potential field on a grid (it has periodic boundary  
> conditions), and I want to calculate the acceleration (force field) of  
> this, i.e.,  $f = -\text{grad}(\text{potential})$ , I need the gradient of the potential .  
> I wrote a procedure, but it has too many for loops in it. Does anybody  
> know a fast and smart way to do this?  
> Thanks!!  
>  
> Andres

Assuming that you are happy with first-order, centered differences, you want something like this

```
grad_x = (SHIFT(phi, -1, 0) - SHIFT(phi, 1, 0))/(2.0*dx)
grad_y = (SHIFT(phi, 0, -1) - SHIFT(phi, 0, 1))/(2.0*dy)
```

where phi is the potential. I think this handles the periodic boundary conditions properly, but check to make sure.

Cheers, Ken Bowman

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