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| No. | Reviewer One’s Comment | Action taken |
| 1. | The paper would be improved if the work were better motivated by an example application near the start of the paper (for example, the MD simulation that is used later in the paper). | We mentioned the example application used and referenced it in the introduction. |
| 2. | There needs to be an explanation of why the temperature needs to be exchanged between replicas and what the role of the Metropolis algorithm is. | We explained and referenced this in section 2 (a). |
| 3. | In Figure 4, shouldn't the x-axis be labeled "Number of machines"? | Corrected this mistake. |
| 4. | When multiple replicas are concurrently searching for a partner to exchange with it is not clear how this is done safely. Even with reverification non-deterministic behavior could still arise if care is not taken. | The replicas are matched using the Metropolis scheme, which is non-deterministic. We explained this in section 3 (b) (ii). |
| 5. | 1) Don't use symbols to refer to "Section" - write it out as text. 2) Try to avoid using the word "utilize" and derivatives thereof. The word "use" can almost always be used instead. 3) Introduction, line 1, change to "Replica-Exchange (RE)......methods represent a class of algorithms..." 4) Introduction, first para: Change "developed against" to "developed within"? 5) Introduction, near end of second para: remove "different coordination mechanisms". 6) Section 2(a), line 3: change to "total time-to-completion of an experiment". 7) Don't use ampersand - use "and" instead. 8) 3 lines after eqn. 2.2: this is the first mention of the advert server, so you either need to explain what it is, or make a forward reference, or drop the text in parentheses. Also "book-keeping" should be "bookkeeping". 9) Last line of page 2: change to "in the asynchronous-centralised case". 10) Section 2(b), second para, line 1: change to "For the synchronous RE formulation". 11) Section 2(b), third para: omit comma after "consequence". 12) Section 2(b), fourth para, line 1: omit "there are". 13) Section 3(a), first para, last line: change "the conduction of" to "conducting". 14) Section 3(a), second para, line 2: change to "enables the dynamical use of a range of" 15) Section 3(a), third para, change "store which is used for" to "store used for". 16) Section 3(a), third para, line 6: change to "multiple big-jobs". 17) Section 3(b), second para, line 5: change to "has a centralised". 18) Section 3(b)(ii), second para, line 6/7: change | Fixed the typos. |
| to "still in the done state". 19) Section 4, first para, line 3: change to "as well as a basic" 20) Section 4(b), first para, line 2: change to "is in the synchronisation" 21) Section 4(b), third para, line 9: change to "suggests there are between 2 and 4" 22) Section 4(b), third para, line 11: change to "increasing numbers of replicas". 23) Section 4(c), first para, last line: change to "in these cases" 24) Section 5(a), first para, last line: "the" is repeated" 25) Section 5(a), second para, line 2: change to "exchanges to replicas" 26) Section 5(a), last para, last line: "the" is repeated" 27) Section 5(b), first para, line 1: change to "of the asynchronous" 28) Section 6, first para, line 1: change to "Following theoretical underpinnings (Li and Parashar 2007, Gallicchio et al. 2008), in this paper..." 29) Section 6, second para, line 2: change "enable" to "enables" 30) Section 6, second para, line 5: change "out weight" to "outweigh". |

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| No. | Reviewer Two’s Comments | Action Taken |
| 1. | It would be useful for the authors to compare the replica exchange application, as disussed here, with the general class of "parameter sweep" application -- where some synchronisation may also be required. | We compared the applications in section 2 (b). |
| 2. | The time calculation in equation 2.2 needs further elaboration. Parameters such as T\_ex, T\_mgmt are not clear. For instance, the mention of an "advert-server" is surely an implementation detail? In particular, the authors should comment on whether such a simple linear combination is an effective representation of reality -- given that many of these operations are being performed over a distributed environment. | We changed the terminology/symobols used and explained the equation better. Removed reference to advert-server from this section. We explained the effect of distribution on the terms in equation 2.2 in section 5 (b). |
| 3. | What is the "Metropolis scheme" -- give reference or explain. | We did this in section 2(a). |
| 4. | The advert service (in section 3(a)) needs further discussion. What is an advert in this context. Also how is a key/value pair generated. What does it mean in this context. Is this similar to a DHT in a peer-2-peer system? In particular, the authors should explain how a job is described -- and subsequently matched. |  |
| 5. | In section 3b(ii) -- what is "MD"? It seems that even in the decentralized case, the advert service is still centralized? Are there issues of latency when accessing the advert service or keeping it consistent? |  |